CCC-629

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U.S. DEPARTMENT OF ENERGY

RSICC COMPUTER CODE COLLECTION

SESOIL

Code System to Calculate One-Dimensional Vertical Transport for the Unsaturated Soil Zone

Contributed by:

Oak Ridge National Laboratory
Oak Ridge, Tennessee
and
Wisconsin Department of Natural Resources
Madison, Wisconsin

RADIATION SAFETY INFORMATION COMPUTATIONAL CENTER

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1. NAME AND TITLE

SESOIL: Code System to Calculate One-Dimensional Vertical Transport for the Unsaturated Soil Zone.

2. CONTRIBUTORS

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Wisconsin Department of Natural Resources, Madison, Wisconsin.

3. CODING LANGUAGE AND COMPUTER

FORTRAN 77; IBM PC's and compatibles. (C00629/IBMPC/02)

4. NATURE OF PROBLEM SOLVED

SESOIL, as an integrated screening-level soil compartment model, is designed to simultaneously model water transport, sediment transport, and pollutant fate. SESOIL is a one-dimensional vertical transport model for the unsaturated soil zone. Only one compound at a time can be considered. The model is based on mass balance and equilibrium partitioning of the chemical between different phases (dissolved, sorbed, vapor, and pure). The SESOIL model was designed to perform long-term simulations of chemical transport and transformations in the soil and uses theoretically derived equations to represent water transport, sediment transport on the land surface, pollutant transformation, and migration of the pollutant to the atmosphere and groundwater. Climatic data, compartment geometry, and soil and chemical property data are the major components used in the equations. SESOIL was developed as a screening-level model, utilizing less soil, chemical, and meteorological values as input than most other similar models. Output of SESOIL includes time-varying pollutant concentrations at various soil depths and pollutant loss from the unsaturated zone in terms of surface runoff, percolation to the groundwater, volatilization, and degradation. The version of SESOIL in RSIC's collection runs stand alone and is functionally equivalent to the version in the RISKPRO system distributed and supported by General Sciences Corporation. The February 1995 release corrected an error that caused the code to fail when average monthly air temperature was -10C and includes an improved iteration procedure for the mass balance equations in the model. In June 1996 a minor change was made to the Fortran source file to correct erroneous values which were sometimes written to the printed output for the user-specified, pollutant mass input table.

5. METHOD OF SOLUTION

The processes modeled by SESOIL are categorized into three cycles: hydrology, sediment, and pollutant transport. Each cycle is a separate sub-model within the SESOIL code. The hydrologic cycle is one-dimensional, considers vertical movement only, and focuses on the role of soil moisture in the soil compartment. The hydrologic cycle is an adaptation of the water balance dynamics theory of Eagleson (1978) and can be described as a dimensionless analytical representation of water balance in the soil column. An iteration technique is used to solve the mass balance equations in the hydrologic cycle. The sediment cycle is optional; it can be turned on or off by the user. If used, SESOIL employs the theoretical sediment yield model EROS (Foster et al., 1980), which considers the basic processes of soil detachment, transport, and deposition. The pollutant fate cycle focusses on the various chemical transport and transformation processes which may occur in the soil and uses calculated results form the hydrologic and sediment washload cycles. The ultimate fate and distribution of the contaminant is controlled by the processes interrelated by a mass balance equation for each soil layer (compartment) that is specified by the user. An iteration procedure is used to solve each equation. The soil compartment is a cell extending from the surface through the unsaturated zone to the upper level of the saturated soil zone, also referred to as the aquifer or groundwater table.

6. RESTRICTIONS OR LIMITATIONS

As many years as desired can be specified for computation using the model. Available storage for the output file is the only limitation in this regard.

Care should be taken when applying SESOIL to sites with large vertical variation in soil properties since the hydrologic cycle assumes a homogeneous soil profile.

7. TYPICAL RUNNING TIME

As an example, a ten-year simulation that includes all four layers with three sublayers per layer requires approximately 5.5 minutes to run and about 250000 bytes of storage on an IBM compatible 486 PC (50 mhz). The author's executable ran in 4 minutes 21 seconds on a Northgate 486/66 using the included sample input data.

8. COMPUTER HARDWARE REQUIREMENTS

Requirements include an IBM PC or compatible with minimum available RAM of 355 K and minimum available disk space of 1.25 MB for the code and generated output from the sample case.

9. COMPUTER SOFTWARE REQUIREMENTS

The RM Fortran compiler, Version 3.10.01, was used to create the executables included in package. SESOIL was tested at RSIC using the included sample input files on a Northgate 486/66 running MS-DOS 6.2 using RM FORTRAN V2.4 and the MS Linker. This executable can be run as a DOS program from Windows 95.

10. REFERENCES

a: Included in documentation:

D. M. Hetrick, "Instructions for Running Stand-Alone SESOIL Code" (October 1993).

D. M. Hetrick, "Background Information on February 1995 Modifications to SESOIL" (January 21, 1994).

D. M. Hetrick, S. J. Scott, with M. J. Barden "The New SESOIL User's Guide," PUBL-SW-200-93 (Revision 1.6) (August 1994).

b: Background information:

M. Bonazountas and J. Wagner (Draft), "SESOIL: A Seasonal Soil Compartment Model." Arthur D. Little, Inc., Cambridge, MA, prepared for the U.S. Environmental Protection Agency, Office of Toxic Substances, (1981, 1984). (Available through National Technical Information Service, publication PB86-112406).

P. S. Eagleson, "Climate, Soil, and Vegetation." Water Resources Research 14(5):705-776, (1978).

G. R. Foster, L. J. Lane, J. D. Nowlin, J. M. Laflen, and R. A. Young, "A Model to Estimate Sediment Yield from Field-Sized Areas: Development of Model." Purdue Journal No. 7781 (1980).

11. CONTENTS OF CODE PACKAGE

The referenced documents in 10a. and 1 DS/HD (1.44 MB) diskette are included. The diskette written in DOS format contains the SESOIL source code, sample input and output data, and the author's executable.

12. DATE OF ABSTRACT

August 1994, February 1995, September 1995, July 1996.

KEYWORDS: HYDRODYNAMICS; MICROCOMPUTER

SECTION 1

Instructions for running stand-alone SESOIL code (version October, 1993)

The source code for the new SESOIL program is named SESOIL.NEW and is provided on the accompanying diskette. The executable is named SESOIL.EXE. Six data files are required to run the stand-alone version of SESOIL (washload, climate, soil, chemical, application, and executive data files). In the example provided, these files are named WASHWI.INP, CLIMWI.INP, SOILWI.INP, CHEMWI.INP, APPLWI.INP, and EXECWI.INP (these files describe an application in the state of Wisconsin). All data in these files are in fixed format. That is, if new files are created that obtain other site-specific data, the new data must be in the same columns that contain the data in these example files. It is suggested that the user copy the existing files to new file names and edit the new files (with user-supplied editor) to replace "old" data with "new" data, being careful to always keep the data in the same columns as before.

The parameters in the files are described in detail in the new SESOIL user's manual (Hetrick and Scott, 1993), with the exception of new parameters needed for two additional options added to the model (SAIC, 1994), and the parameters in the executive data file (EXECWI.INP). Data for the two new options are in the application data file (APPLWI.INP), and are controlled by two switches named ISUMRS and ICONC (see line 2 of APPLWI.INP). These switches have the following definitions (note that the new SESOIL user's manual contains an example that does not include these new options):

ISUMRS = switch to determine if Summers model (Summers, Gherini, and Chen, 1980) is used to compute contaminant concentration in the saturated zone below the unsaturated column of SESOIL (1 for YES, 0 for NO).

ICONC = switch to determine if initial concentrations for each sublayer are input to SESOIL (1 for YES, 0 for NO).

If ISUMRS = 1, the following parameters are needed in the application data file (see APPLWI.INP):

SATCON = saturated hydraulic conductivity (cm/d),
HYDGRA = hydraulic gradient (-),
THICKS = thickness of saturated zone (cm),
WIDTH = width of contaminated zone perpendicular to the groundwater flow (cm), and
BACKCA = background concentration of the contaminant in the aquifer (µg/ml).

Note that if ISUMRS = 0, then the two lines containing these Summers parameters would not appear in the application data file (see APPLWI.INP).

If ICONC = 1, the following parameters are needed in the application data file (see APPLWI.INP):

IMONCN = month of year to load initial concentrations (1.0 = month of October), and
CONCIN(I,J) = initial concentrations in µg/ml for layer I (I=1,ILYS), sublayers J=1,NSUBL(I)

where ILYS is the number of major soil layers (given in line 2 of the application file), and NSUBL(I) is the number of sublayers for each major layer I (given in line 3 of the application file).

Note that if ICONC=0, the six lines containing the parameters IMONCN and CONCIN(I,J) would not appear in the application data file (see APPLWI.INP).

The new SESOIL user's manual describes the use of SESOIL in the RISKPRO™ system, an information management tool designed to help users perform exposure assessments (General Sciences Corporation, 1990). RISKPRO™ creates the executive data file (EXECWI.INP) for you and thus the contents of this file are not described in the new user's manual. However, this file is described in the original SESOIL user's manual by Bonazountas and Wagner (1984), available as publication PB86-112406 from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161. The parameters in this file are defined as follows:

RUN = incremental number of the run.
OPTN = simulation option (the monthly option M is suggested).
CLIM = the index for the climate data (corresponds to the number on the first line of data for the climate at the site; see the climate data file CLIMWI.INP).
SOIL = the index for the soil data (corresponds to the number on the first line of data for the particular soil type at the site; see the soil data file SOILWI.INP).
CHEM = the index for the chemical data (corresponds to the number on the first line of data for the particular chemical of interest; see the chemical data file CHEMWI.INP).
WASH = the index for the washload data (corresponds to the number on the first line of data for the washload parameters at the site; see the washload data file WASHWI.INP). Set WASH to 0 if the washload is to be ignored.
APPL = the index for the application area (corresponds to the number on the first line of data for the site application parameters; see the application data file APPLWI.INP).
YRS = the number of years to be simulated for the run.

Multiple runs are specified with multiple run/line entries in the executive data file. The last line contains 999 to indicate the end of the file.

To run the stand-alone SESOIL code on an IBM compatible PC using the example data files included in this package, simply use the batch file SESOILWI.BAT. By typing SESOILWI and the enter key, SESOIL will run using the data in files WASHWI.INP, CLIMWI.INP, SOILWI.INP, CHEMWI.INP, APPLWI.INP, and EXECWI.INP. The results file from a run will always be named FORT21; the user should rename this file between runs. To use new data in different file names, simply copy the batch file SESOILWI.BAT to a new name with the .BAT extension, edit the batch file to include the names of the new data files, and run by typing the new batch file name and the enter key.

References

Bonazountas, M., and Wagner, J., *SESOIL: A Seasonal Soil Compartment Model*, Arthur D. Little, Inc., Cambridge, Massachusetts, prepared for the U.S. Environmental Protection Agency, Office of Toxic Substances, 1984. (Available through the National Technical Information Service, publication PB-112406).

General Sciences Corporation, Inc., *RISKPRO User's Guide*, General Sciences Corporation, Laurel, Maryland, 1990.

Hetrick, D.M. and Scott, S.J., *The New SESOIL User's Guide*, Wisconsin Department of Natural Resources, PUBL-SW-200, Madison, WI, 1993.

Science Applications International Corporation (SAIC), *Vadose Zone Soil Leaching Report*, DOE/OR/12-1249&D0, POEF-ER-4591&D0, 11197 U.S. Route 23, Suite 200, Waverly, Ohio 45690.

Summers, K., Gherini, S., and Chem, C., *Methodology to Evaluate the Potential for Groundwater Contamination from Geothermal Fluid Release*, EPA-600/7-80-117, as modified by U.S. EPA Region IV, 1980.

SECTION 2

SOFTWARE REQUIREMENTS RECORD

GENERAL OVERVIEW: Refer to the new User's Manual for SESOIL, Sections 1-3 (Hetrick, Scott, and Barden, 1993) for a general overview of the purpose of the SESOIL model, including all assumptions and techniques employed. Two new options that have been added to SESOIL for this study include: (1) adding the capability to input an initial concentration for each sublayer of up to four major layers (could only input loading for each major layer previously), (2) adding an option to include the saturated zone below the unsaturated column of SESOIL. A modified Summer's model equation (Summers, Gherini, and Chem, 1980) will be used for computing the contaminant concentration in the saturated zone.

INPUTS: For the original SESOIL, all inputs, including formats and valid ranges, are thoroughly described in the User's Manual (Section 4). If data are input incorrectly to SESOIL, error or warning messages are printed by the code. These messages are explained in Appendix C of the User's Manual (Hetrick, Scott, and Barden, 1993).

For the new options that were added, input parameters required are:

ICONC = switch to determine if initial concentrations for each sublayer are input (1 for YES, 0 for NO)

IMONCN = month of year to load initial concentrations (only used if ICONC = 1).

CONCIN(I) = initial concentrations for sublayers I=1,NSUBT where NSUBT is the total number of sublayers (ug/ml) (only used if ICONC = 1).

ISUMRS = switch to determine if Summer's model (Summers, Gherini, and Chem, 1980) is used to compute contaminant concentration in the saturated zone (1 for YES, 0 for NO).

Following parameters are needed if ISUMRS = 1:

SATCON = saturated hydraulic conductivity (cm/d).

HYDGRA = hydraulic gradient (-).

THICKS = thickness of saturated zone (cm).

WIDTH = width of contaminated zone perpendicular to the groundwater flow (cm).

BACKCA = background concentration of the contaminant in the aquifer (ug/ml).

PROCESSING: All specific operations are described in the SESOIL User's Guide (Section 3) with the exception of the two new options (see General Overview above). The code checks for invalid input data and prints error or warning messages if abnormal situations are recognized. Also, all the input data are printed in the output file of SESOIL so that the data can be checked. This is true for the two new options that were added. If ISUMRS = 1, the equation used to compute the concentration of the contaminant in the saturated zone C_{gw} (ug/ml) is (Summers, Gherini, and Chem, 1980):

$$C_{gw} = (Q_p C_l + Q_a C_a)/(Q_p + Q_a)$$

where

Q_p = volumetric flow rate of infiltration (soil pore water) into the aquifer (cm^3/d) (this value is provided by SESOIL).

Q_a = volumetric flow rate of groundwater beneath the waste area (cm^3/d). Q_a is computed by the modified SESOIL as:

$$Q_a = SATCON*HYDGRA*THICKS*WIDTH$$

C_l = contaminant concentration in the soil pore water before entering the aquifer (ug/ml) (this value is provided by SESOIL).

C_a = BACKCA (input parameter).

OUTPUTS: All outputs from the SESOIL model are described in Section 5 of the SESOIL User's Guide (Hetrick, Scott, and Barden, 1993). All error or warning messages that are printed by SESOIL during execution are described in Appendix C of the manual. If the modified Summer's model option is used, then C_{gw} is printed for each month once the contaminant has reached the groundwater. The accuracy of the output is dependent on the accuracy of the input data and proper use of the model. Calibration of the hydrology of the model to measurements at the site will be done wherever possible.

EXTERNAL INTERFACE REQUIREMENTS: SESOIL has been linked (Hetrick, Luxmoore, and Tharp, 1993) to the Latin hypercube sampling model PRISM (Gardner, Rojder, and Berstrom, 1983; Gardner, 1984). In PRISM, all the input distributions for key soil, chemical, and climate parameters for SESOIL are divided into N equal probability classes (200, for example). These distributions are sampled to generate N input data sets. PRISM runs the SESOIL model for each set of parameter values, resulting in model predictions for each set. The joint set of model parameters and predictions are evaluated statistically by PRISM to indicate the most sensitive parameters for given output variables. Output frequency distributions for selected SESOIL components are produced. The requirements for the SESOIL/PRISM interface are described in Hetrick, Luxmoore, and Tharp (1993).

REFERENCES

Gardner, R.H., B. Rojder, and U. Berstrom, PRISM, A systematic method for determining the effect of parameter uncertainties on model predictions, Studsvik Energiteknik AB report NW-83/555, Nykoping, Sweden, 49 pp., 1983.

Gardner, R.H., A unified approach to sensitivity and uncertainty analysis, Proc. of the tenth IASTED International Symposium: Applied Simulation and Modeling, San Francisco, California, pp. 155-157, 1984.

Hetrick, D.M., R.J. Luxmoore, and M.L. Tharp, Latin hypercube sampling with the SESOIL model, Eighth Annual Conference: Hydrocarbon Contaminated Soils - Analysis, Fate, Environmental & Public Health Effects, Remediation, and Regulatory Issues, Amherst, Massachusetts 01003, September 19-23, 1993.

Hetrick, D.M., S.J. Scott, and M.J. Barden, The New SESOIL User's Guide, PUBL-SW-200-93, Wisconsin Department of Natural Resources, Madison, WI 53707, 125 pp., 1993.

Summers, K., S. Gherini, and C. Chem, Methodology to evaluate the potential for groundwater contamination from geothermal fluid release, EPA-600/7-80-117, as modified by EPA Region IV, 1980.

SECTION 3

The New SESOIL User's Guide

David M. Hetrick
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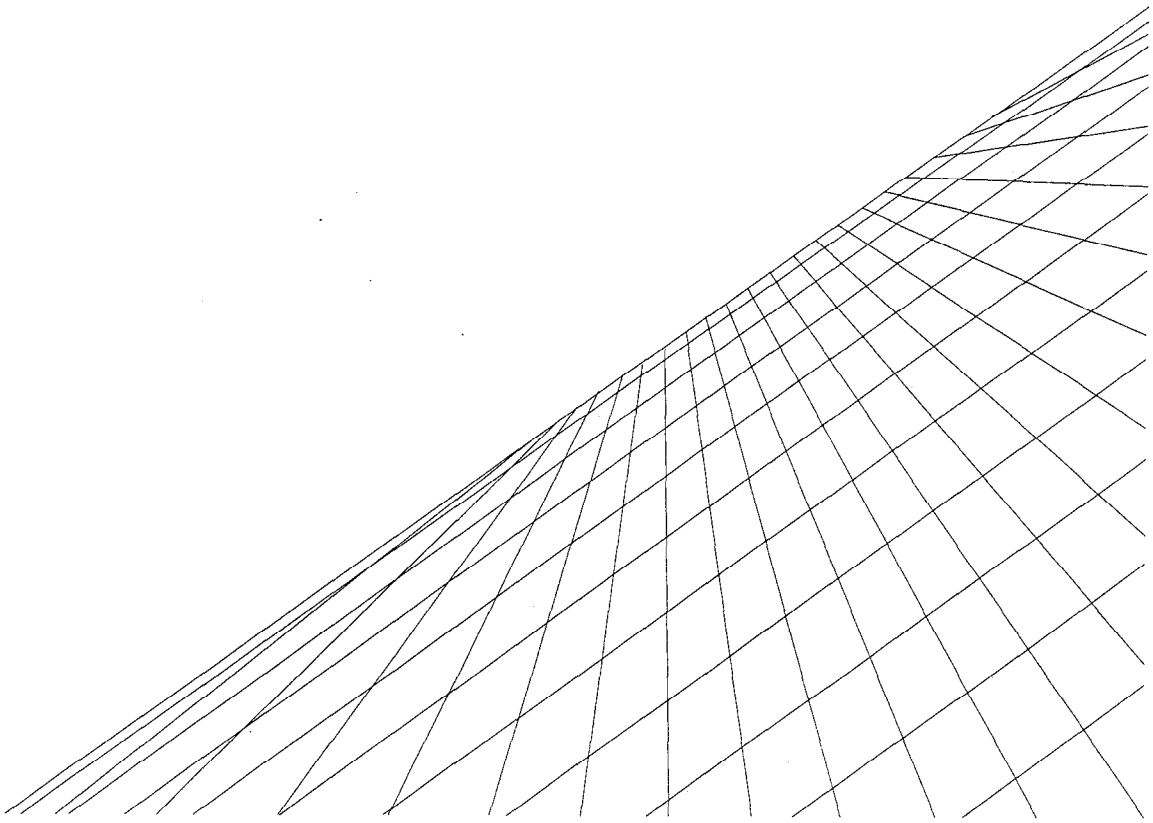

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The New SESOIL User's Guide

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Since original documentation of the EPA's SESOIL manual was outdated due to numerous changes made to the model over the years , the WDNR decided to fund an easier to use SESOIL manual for its Department personnel and the regulated community. This manual provides the technical and non-technical user with a better understanding of how the SESOIL model works and how it can be applied in real world situations.

As part of the GCSE project, the SESOIL model (an unsaturated soil zone transport computer model) was to be used by WDNR to evaluate factors affecting the movement of organic compounds in unsaturated soil environments found typically in Wisconsin, and to estimate residual contamination levels (RCL's) for particular compounds.

The authors wish to especially thank Carol McCurry and Mike Barden from the WDNR for their support and visionary views of computer technology in environmental risk assessment. In addition, the authors also wish to thank Ken Ladwig of STMI and the General Science Corporation for all their support during the development of this manual.

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1 Introduction Overview of the SESOIL Model

SESOIL is an acronym for Seasonal Soil Compartment Model and is a one-dimensional vertical transport code for the unsaturated soil zone. It is an integrated screening-level soil compartment model and is designed to simultaneously model water transport, sediment transport, and pollutant fate. The program was developed for EPA's Office of Water and the Office of Toxic Substances (OTS) in 1981 by Arthur D. Little, Inc. (ADL). ADL updated the SESOIL model in 1984 to include a fourth soil compartment (the original model included up to three layers) and the soil erosion algorithms (Bonazountas and Wagner, 1984). A comprehensive evaluation of SESOIL performed by Watson and Brown (1985) uncovered numerous deficiencies in the model, and subsequently, SESOIL was modified extensively by Hetrick et al. at Oak Ridge National Laboratory (ORNL) to enhance its capabilities (see Hetrick et al., 1986, 1988, 1989). The model is designed to be self-standing, but SESOIL was incorporated into a system called PCGEMS (Graphical Exposure Modeling System for the PC), a complete information management tool developed for EPA-OTS and designed to help users perform exposure assessments (General Sciences Corporation, 1987, 1989). Subsequently, PCGEMS was turned into the system called RISKPRO; which has numerous additions and improvements to PCGEMS, and is fully supported (General Sciences Corporation, 1990). The purpose of this document is to provide an up-to-date users manual for SESOIL as it is used in the RISKPRO system.

Side Note: The SESOIL program is written in the FORTRAN language.

SESOIL was developed as a screening-level model, utilizing less soil, chemical, and meteorological values as input than most other similar models. Output of the SESOIL model includes time-varying pollutant concentrations at various soil depths and pollutant loss from the unsaturated zone in terms of surface runoff, percolation to the groundwater, volatilization, and degradation.

The SESOIL model accepts time-varying pollutant loading. For example, it is able to simulate chemical releases to soil from a variety of sources such as landfill disposal, accidental leaks, agricultural applications, leaking underground storage tanks, or deposition from the atmosphere. Other potential applications of SESOIL include long term leaching studies from waste disposal sites, pesticide and sediment transport on watersheds, studies of hydrologic cycles and water balances of soil compartments, and precalibration runs for other simulation models. One may also run the model to estimate the effect of various site management or design strategies on pollutant distributions and concentrations in the environment.

SESOIL can be used as a screening tool in performing exposure assessments. OTS used the model to predict the behavior of pollutants in soil compartments for analyzing and prioritizing chemical exposures. A number of studies have been conducted on the SESOIL model including sensitivity analysis, comparison with other models, and comparisons with field data (Bonazountas et al., 1982; Wagner

et al., 1983; Hetrick, 1984; Kincaid et al., 1984; Watson and Brown, 1985; Hetrick et al., 1986; Melancon et al., 1986; Hetrick et al., 1988; Hetrick et al., 1989). SESOIL has been applied in risk assessments concerning direct coal liquefaction (Walsh et al., 1984), incineration of hazardous waste (Holton et al., 1985; Travis et al., 1986), the transport of benzene to groundwater (Tucker et al., 1986), to soil cleanup levels in California (Odencrantz et al., 1991, 1992), and to site sensitivity ranking for Wisconsin soils for the Wisconsin Department of Natural Resources (Ladwig et al., 1992).

The soil column in SESOIL is a user-defined compartment extending from the surface through the unsaturated zone to the groundwater table. Typically, SESOIL is used to estimate the rate of migration of chemicals through soils and the concentration of the chemical in soil layers following chemical release to the soil environment. SESOIL's simulation of chemical persistence considers mobility, volatility, and degradation. The model performs calculations on an annual or monthly basis, and can simulate up to 99 years of chemical transport.

The model requires several types of chemical- and site-specific data to estimate the concentration of the chemical in the soil, its rate of leaching toward groundwater, and the impact of other environmental pathways. The user is required to provide chemical properties and release rate, and soil and climate data. This user's guide is designed to provide users of SESOIL with the information needed to efficiently and appropriately run the model and interpret the results. It provides a brief overview of how SESOIL can be used as an assessment tool. This document discusses the assumptions and equations used in the model and describes the use of SESOIL in the RISKPRO system, including details on how to build the input data files. A complete discussion of the output data file from SESOIL and the graphing capabilities available in the RISKPRO system is provided.

1.1 The RISKPRO System

The RISKPRO system simplifies data input by providing interactive prompts, parameter menus, and data retrieval programs in order for the user to extract pertinent data from on-line databases, create the input files required by SESOIL, run the model, and review and graph the model results.

☐ ***Side Note:***
Although the math co-processor is not required, it is highly recommended since it substantially reduces computer time.

The minimum system requirements for RISKPRO are:

- IBM XT/AT/PS2, 80386 or compatibles with 640 K RAM
- Hard Disk and 1 floppy disk drive
- DOS Version 2.2 or higher
- Graphics display adapter
- 540 K RAM available at all times
- 8087, 80287, or 80387 Math Co-processor.

Exposure Assessment Overview

2

Concerns regarding actual and potential environmental pollution have made it necessary to know the fate and transport of chemicals entering the soil environment. For example, a synthetic, organic chemical may find its way into the soil and eventually to the groundwater from an unlined disposal site or a leaking underground storage tank. To better understand the possible impact of a chemical in the environment, one needs to develop a methodology that can predict where in the environment a chemical substance will be transported, and the rate and extent of its transformations.

In order to help define the impacts that chemical releases could have on the environment and human exposure, the SESOIL model can be used to perform an exposure assessment. In using the SESOIL model as an assessment tool, the first step involves information gathering. The essential information includes:

- **the behavior of the chemical in the environment**
- **the rate and frequency of its release into the environment**
- **a description of the media in which the chemical is released.**

In the SESOIL scenario, simulation of a chemical release to the land would include detailed information about the soil, the chemical, local weather patterns, and the underlying aquifers.

This manual will show the reader how to use the SESOIL model to determine the concentration of a chemical in various layers of the soil, including the surface layer. The SESOIL model can be used as an assessment tool to help the user estimate the volatilization of the chemical to the atmosphere, runoff rates, chemical concentrations in the soil column, and the rate of vertical migration (leaching) of a chemical toward groundwater, including quantities entering the groundwater.

SESOIL Model Description

3

SESOIL is a one-dimensional vertical transport model for the unsaturated soil zone. SESOIL can consider only one compound at a time and the model is based on mass balance and equilibrium partitioning of the chemical between different phases (dissolved, sorbed, vapor, and pure). The SESOIL model was designed to perform long-term simulations of chemical transport and transformations in the soil. The model uses theoretically derived equations to represent water transport, sediment transport on the land surface, pollutant transformation, and migration of the pollutant to the atmosphere and groundwater. Climatic data, compartment geometry, and soil and chemical property data are the major components used in the equations.

The expression "long term" applies to both annual and monthly simulations in SESOIL, and is used in contrast to "short-term" models which employ a storm-by-storm resolution. Some soil models are designed to estimate pollutant distribution in the soil after each major storm event, and simulate chemical concentrations in the soil on a daily basis (e.g., see Patterson et al., 1984). These models are data intensive, requiring, for example, hourly rainfall input and daily maximum and minimum temperatures. SESOIL, on the other hand, estimates pollutant distribution in the soil column and on the watershed after a "season", which can be defined by the user as a year or a month. This is accomplished using a statistical water balance analysis and a washload routine statistically driven within the season. This approach saves time for the model user by reducing the amount of data that must be provided, and also reduces computer time and resource requirements since fewer computations are required.

☐ ***Side Note:***
The SESOIL model is not data intensive.

Two operation options are available for running SESOIL: annual estimates (Option A) requiring annual climatic data, and monthly estimates (Option M) requiring monthly data. It is recommended that the monthly option always be selected as it will provide a better estimate of chemical movement through the soil. RISKPRO simplifies the task of compiling monthly input data by extracting pertinent data from on-line databases (see the next section on building input data files using RISKPRO). Thus, the monthly option is no more difficult to use than the annual option. Option A is not available in the RISKPRO system, and this option will not be discussed further in this report with the exception of the hydrologic cycle, which implements the annual algorithm as described below. The annual option has not been changed from the original model, and those users interested in the annual option are referred to the report by Bonazountas and Wagner (1984).

The processes modeled by SESOIL are categorized into three cycles: hydrology, sediment, and pollutant transport. Each cycle is a separate sub-model within the SESOIL code. Most mathematical environmental simulation models may be categorized as stochastic or deterministic models. Both the stochastic and deterministic models are theoretically derived. Stochastic models incorporate the

concept of probability or some other measure of uncertainty, while deterministic models describe the system in terms of cause/effect relationships. SESOIL employs a stochastic approach for the hydrologic and washload cycles, and a deterministic approach for the pollutant transport cycle.

3.1 The Soil Compartment

In SESOIL, the soil compartment (or column) is a cell extending from the surface through the unsaturated zone to the upper level of the saturated soil zone, also referred to as the aquifer or groundwater table. While SESOIL estimates the pollutant mass added to the groundwater, the saturated zone is not modeled. The output from SESOIL can be used for generating input values for groundwater transport models. (In RISKPRO, the Analytic Transient 1-2-3 Dimensional Model, AT123D (Yeh, 1981), has been adapted to use SESOIL results for groundwater runoff (recharge) to simulate chemical movement in the saturated zone.)

Side Note:
Two to four layers and up to 40 sublayers, 10 in each layer, can be specified.

The soil compartment is treated differently by the hydrologic cycle and the pollutant cycle in SESOIL. In the hydrologic cycle, the whole soil column is treated as a single homogeneous compartment extending from the land surface to the water table. The pollutant cycle breaks the soil column into several compartments, also called layers. The layers in the pollutant cycle can be further broken up into sublayers. Each soil layer (sublayer) is considered as a compartment with a set volume and the total soil column is treated as a series of interconnected layers (sublayers). Each layer (sublayer) can receive and release pollutant to and from adjacent layers (sublayers).

The dimensions of the soil compartment are defined by the user. The width and length of the column are defined as the area of application of pollutant released to the soil, and the depth to the groundwater is determined from the thickness of user-defined soil layers that are used in the pollutant cycle. The soil column can be represented in 2, 3, or 4 distinct layers. Up to 10 sublayers can be specified for each layer, each having the same soil properties as the layer in which they reside.

There is no optimal size for the soil layers (sublayers); the dimensions of the soil column can be specified to cover any area from one square centimeter to several square kilometers. The area of the compartments is important for mass balance, but in terms of pollutant concentration the area of application is irrelevant since it is constant for all layers (sublayers). Note that the equations in SESOIL have been normalized to an area of one square centimeter.

It is suggested that the minimum depth of a layer is one centimeter. Depending on the application, layer depths can range from a shallow root zone of 5-25 centimeters, to a deep layer of more than 10 meters. When the pollutant enters a layer (sublayer), the model assumes instantaneous and uniform distribution of the chemical throughout that layer (sublayer). The model performs mass balance calculations over each entire soil layer (sublayer); there is no concentration gradient within a layer (sublayer). For a given amount of chemical released, the larger the layer (sublayer), the lower the calculated chemical concentration. For

this reason, SESOIL was discretized to allow as many as ten sublayers in each of the four possible major layers. Thus, the user may define as many as 40 smaller compartments using these sublayers. The result is an increase in the resolution of the model.

3.2 SESOIL Cycles

Pollutant transport and transformation in the unsaturated soil zone are complex processes affected by chemical, soil, and hydrogeological properties. In SESOIL, these processes are included in one of three cycles: the hydrologic cycle to deal with moisture movement or flow through the compartment, the sediment or washload cycle to deal with runoff from the soil surface, and the pollutant fate cycle. SESOIL was developed by integrating three submodels, one to deal with each cycle. The specific processes associated with each cycle are accounted for in the submodels. The cycles and their associated processes are summarized in Table 3.1 and Diagram 1 shows a schematic of the soil column.

The hydrologic cycle is done first in SESOIL, followed by the sediment cycle, and these results are used in the pollutant fate cycle. The hydrologic cycle is based on a statistical, dynamic formulation of a vertical water budget. It has been adapted to account for either yearly or monthly simulations and for moisture variations in the soil. The hydrologic cycle controls the sediment cycle, which is a theoretical monthly washload routine. The pollutant cycle simulates transport and transformation processes in three phases present in the soil compartment: soil-air or gaseous phase, soil-moisture phase, and adsorbed or soil-solids phase. The three major cycles are summarized in the sections that follow.

Table 3.1
SESOIL CYCLES

Hydrologic Cycle

- Rainfall
- Infiltration
- Groundwater runoff (recharge)
- Surface runoff
- Capillary rise
- Evapotranspiration
- Soil moisture retention (storage)

Sediment Cycle

- Sediment washload (erosion due to storms)

Pollutant Fate Cycle

- Advection
- Cation exchange
- Diffusion (air phase)
- Volatilization
- Sorption
- Hydrolysis
- Washload
- Surface runoff
- Groundwater runoff (recharge)
- Metal complexation
- Chemical degradation/decay

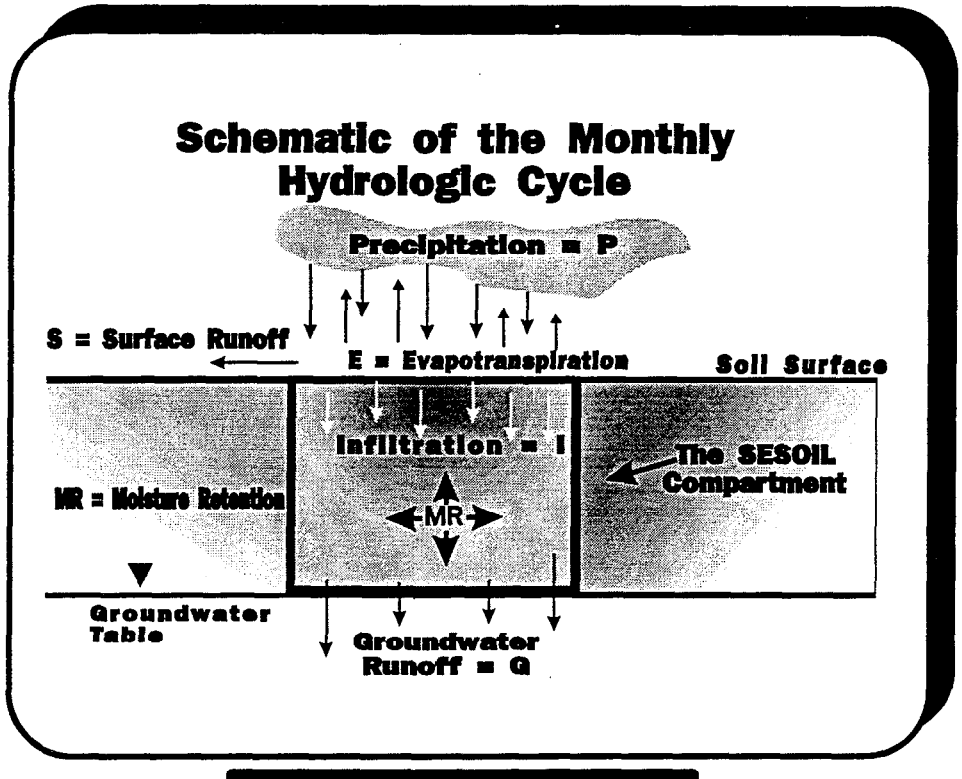
Schematic of the Monthly Hydrologic Cycle
Precipitation = P
S = Surface Runoff
E = Evapotranspiration
Soil Surface
Infiltration = I
The SESOIL Compartment
MR = Moisture Retention
MR
Groundwater Table
Groundwater Runoff = Q

Diagram 1

3.3 Hydrologic Cycle

The hydrologic cycle is one-dimensional, considers vertical movement only, and focuses on the role of soil moisture (or interstitial pore water) in the soil compartment. The hydrologic cycle submodel calculates results for the hydrology of a site and passes these results to both the sediment washload cycle and the pollutant fate cycle. The hydrologic cycle used in SESOIL is an adaptation of the water balance dynamics theory of Eagleson (1978). The theory can be described as a dimensionless analytical representation of an **annual** water balance. It is itself a model based on simplified models of interacting hydraulic processes, including terms for the climate, soil, and vegetation. These processes are coupled through statistically based modeling.

It is beyond the scope of this manual to present the detailed physics and mathematical expressions of the model. The hydrologic cycle is thoroughly described by Eagleson (1978) and summarized by Bonazountas and Wagner (1984), and is based on the water balance equations shown below. All of these parameters are expected or mean annual values, and in SESOIL they are expressed in centimeters.

$$P - E - MR = S + G = Y \qquad (1)$$

$$I = P - S \qquad (2)$$

where:

- P = precipitation
- E = evapotranspiration
- MR = moisture retention
- S = surface runoff
- I = infiltration
- Y = yield
- G = groundwater runoff or recharge (includes term for capillary rise)

Briefly, precipitation is represented by Poisson arrivals of rectangular gamma-distributed intensity pulses that have random depth and duration. Infiltration is

described by the Philip equation (Philip, 1969), which assumes the medium to be effectively semi-infinite, and the internal soil moisture content at the beginning of each storm and inter-storm period to be uniform at its long-term average. Percolation to the groundwater is assumed to be steady throughout each time step of simulation, at a rate determined by the long-term average soil moisture content. Capillary rise from the water table is assumed to be steady throughout the time period and to take place to a dry surface. The work of Penman (1963), Van den Honert (1948), and Cowan (1965) is employed in calculating evapotranspiration (Eagleson, 1978). Surface runoff is derived from the distribution of rainfall intensity and duration, and by use of the Philip infiltration equation. The effects of moisture storage are included in the monthly option in SESOIL, based on the work of Metzger and Eagleson (1980).

Eagleson's theory assumes a one-dimensional vertical analysis in which all processes are stationary in the long-term average. The expression "long term" applies to both annual and monthly simulations in SESOIL, and is used in contrast to "short-term" models which employ a storm-by-storm resolution. Also, Eagleson's approach assumes that the soils are homogeneous and that the soil column is semi-infinite in relation to the surface processes. Thus, in the hydrologic cycle of SESOIL, the entire unsaturated soil zone is conceptualized as a single layer (or compartment) and the prediction for soil water content is an average value for the entire unsaturated zone.

While the user can provide different permeability values as input for each of the four major soil layers for the pollutant cycle in SESOIL, the hydrologic cycle will compute and use the depth-weighted average permeability according to the formula:

$$K_z = \frac{d}{\sum_{i=1}^{n} \frac{d_i}{K_i}} \qquad (3)$$

where:

K_z = vertically averaged permeability (cm^2),

K_i = permeability for layer i (cm^2),

d = depth from surface to groundwater (cm),

d_i = thickness of layer i (cm).

Thus, the user should exercise care when applying SESOIL to sites with large vertical variations in soil properties. The average permeability calculated by Eq. (3) in the hydrologic cycle may not be what the user intended and the resulting computed average soil moisture content may not be valid.

There is no explicit consideration of snow and ice, which are entered as precipitation. The model assumes that the water table elevation is constant with no change in groundwater storage from year to year. Bonazountas et al. (1984) adopted this theory for both annual and monthly simulations.

Each process in Eqs. (1) and (2) is written in terms of the soil moisture content, and solution of the equations is accomplished by iterating on soil moisture until the calculated value for precipitation is within 1.0% of the measured value input by the user. When this iteration is complete, the components such as infiltration, evapotranspiration, etc., in Eqs. (1) and (2) are known. SESOIL uses this procedure in both the annual and monthly routines. The monthly routine is an extension of the annual routine; both are discussed further below.

3.3.1 Annual Cycle

The annual water balance routine is based on Eagleson's (1978) theory. It encompasses one year, so multiple years have to be simulated as separate cycles. This routine simply determines the soil moisture content based on solution to equations (1) and (2) using annual climatic parameters. When the value for soil moisture content is arrived at through the iteration technique, the various processes described in equations (1) and (2) are known. Note that storage effects in the soil are not considered in the annual option. The theoretical basis for the annual dynamic hydrologic cycle used in SESOIL has been validated by Eagleson (1978). Annual model predictions were compared with empirical observations for five years of precipitation data at both a subhumid and arid climate location, with close agreement.

3.3.2 Monthly Cycle

The monthly water balance routine is based on the same theory as the annual routine, with modifications made to the details of moisture transfer from month-to-month (handling of moisture storage), and the radiation effects. The initial value for soil moisture content is calculated in SESOIL by summing the appropriate monthly climatic input data (for the first year) to obtain annual values and using the annual cycle algorithm. Then for **each** month, the monthly input values for precipitation, mean storm number, and mean length of the rain season are multiplied by 12 in order to again obtain "annual" values. Equations (1) and (2) are solved to compute the soil moisture content, and the results for the components (infiltration, evapotranspiration, etc.) are divided by 12 to attain average monthly values.

Note that if long-term average climatic data are used as input for each year (input for each month is the same from year to year), one would expect that the results for the hydrology for each month would be identical from year to year.

However, since the initial soil moisture content is computed as stated above for the first month (of the first year), this value will be different than the soil moisture calculated for the twelfth month that is then used for the first month of the following year. Thus, although hydrology results will not be identical for the first two years, they will be identical thereafter.

The monthly cycle in SESOIL does account for the change in moisture storage from month to month, incorporating the work of Metzger and Eagleson (1980). Also, the SESOIL evapotranspiration algorithm has been modified from the original work of Eagleson (1978) to include seasonal changes in average monthly radiation (radiation was a constant function of latitude before). Hetrick (1984) observed that hydrology predictions of the original SESOIL were insensitive to seasonal changes in meteorological data. To model the hydrology more realistically, an algorithm from the AGTEHM model (Hetrick et al., 1982) which computes daily potential radiation (incoming radiation for cloudless skies) for a given latitude and Julian date (December 31 = 365) is now used. The middle day of the month is used in the algorithm and the effect of cloud cover is calculated with the expression (Hetrick et al., 1982):

$$\bar{S} = S[(1-C) + kC] \qquad (4)$$

where:

- $\bar{S}$ = the average monthly radiation,
- S = the potential radiation,
- C = the fraction of sky covered by clouds, and
- k = the transmission factor of cloud cover.

The value for k used in the model is 0.32, suggested by Hetrick et al. (1982). Since latitude and monthly cloud cover are required input for SESOIL, no new input data are needed to support this modification. There are now more pronounced monthly changes in evapotranspiration predictions (see Hetrick et al., 1986).

Although SESOIL does produce monthly results for soil moisture content of the root zone, defined in the model as the first 100 cm depth from the surface, this option has not been fully developed. Thus, values for soil moisture for the root zone will usually be identical to those for the entire soil column, and only very dry climates may cause a difference (M. Bonazountas, personal communication, 1986).

SESOIL model predictions (using the monthly option) of watershed hydrologic components have been compared with those of the more data intensive terrestrial ecosystem hydrology model AGTEHM (Hetrick et al., 1982) as well as to empirical measurements at a deciduous forest watershed and a grassland

watershed (see Hetrick et al., 1986). Although there were some differences in monthly results between the two models, good agreement was obtained between model predictions for annual values of infiltration, evapotranspiration, surface runoff, and groundwater runoff (recharge). Also, SESOIL model predictions compared well with the empirical measurements at the forest stand and the grassland watersheds.

3.3.3 Hydrologic Model Calibration

Calibration of unsaturated soil zone models can be uncertain and difficult because climate, soil moisture, soil infiltration and percolation are strongly interrelated parameters that are difficult and expensive to measure in the field. However, if at all possible, input parameters for any unsaturated soil zone model should be calibrated so that hydrologic predictions agree with observations. In SESOIL, all input parameters required for the hydrologic cycle can be estimated from field studies with the exception of the pore disconnectedness index, "c". This parameter is defined as the exponent relating the "wetting" or "drying" time-dependent permeability of a soil to its saturated permeability (Eagleson, 1978; Eagleson and Tellers, 1982). Brooks and Corey (1966) presented the following relationship:

$$K(S) = K(1)S^{c} \qquad (5)$$

where:

$K(1)$ = saturated hydraulic conductivity (cm/s),

$K(S)$ = hydraulic conductivity at S (cm/s),

S = percent saturation,

c = pore disconnectedness index.

Thus, this parameter is not commonly found in the literature. Default values for c suggested by Eagleson (1978) and Bonazountas and Wagner (1981, 1984) are: clay 12; silty clay loam 10; clay loam 7.5; silt loam 5.5; sandy loam 6; sandy clay loam 4; and sand 3.7. However, when data are available, this parameter should be varied first to optimize agreement between SESOIL results and hydrologic measurements. It should be noted that most unsaturated soil zone models require detailed data (which are difficult to obtain), such as soil moisture

characteristic curves. The "one variable" approach of Eagleson (1978) simplifies the data estimation process and reduces computational time.

Other sensitive parameters for the hydrologic cycle are the effective porosity and the intrinsic permeability (e.g., see Hetrick et al., 1986, 1989). While other parameters can be varied when calibrating the model to measured hydrologic data, it is recommended that the user vary the disconnectedness index first, followed by the permeability and/or porosity. See the section on input data for further details.

3.4 Sediment Washload Cycle

In pollutant transport models, estimates of erosion and sediment yield on watersheds may be needed in order to compute the removal of sorbed chemicals on eroded sediments. A major factor in this process is the surface runoff, rainwater which does not infiltrate the soil and may carry dissolved pollutant. Surface runoff is computed as part of the hydrologic cycle. Erosion is a function of the rate of surface runoff and several other factors. These factors include the impact of raindrops which detaches soil particles and keeps them in motion as overland flow, surface features such as vegetation and roughness, and infiltration capacity. Because of the difficulty in directly measuring washload using water quality monitoring techniques, estimation techniques and models are widely employed.

The sediment cycle of SESOIL is optional; it can be turned on or off by the user. Thus, if pollutant surface runoff is considered negligible, the washload cycle can be neglected. If the option is used, SESOIL employs EROS, a theoretical sediment yield model (Foster et al., 1980), which is part of the CREAMS model (Knisel, 1980; Foster et al., 1980). The erosion component considers the basic processes of soil detachment, transport, and deposition. The EROS model uses separate theoretically derived equations for soil detachment and sediment transport. Separate equations are needed for these two processes because the relationship of the detachment process to erosion is different than the relationship between erosion and transport.

For the detachment process, the model employs the Universal Soil Loss Equation (USLE) (Wischmeier and Smith, 1978), modified by Foster et al. (1980) for single storm events. The USLE is applicable for predictions of annual sediment erosion originating mainly from small watersheds which are subject to sheet and rill erosion. Detachment of soil particles occurs when the sediment load already in the overland flow is less than the sediment capacity of this flow. The equation takes into account soil erodibility (the rate of soil loss per storm), which varies for different soil types and texture classes. The USLE considers topography, since both the length and the steepness of the land slope affect the rate of rain-induced soil erosion. Also, the land cover (e.g. vegetation) and the roughness of the soil surface affect the rate of erosion and the rate of overland transport. The USLE includes a parameter called "Manning's n", or roughness coefficient, to model these influences.

To model the sediment transport capacity for overland flow, EROS incorporates the Yalin Transport Equation (Yalin, 1963), modified for nonuniform sediment with a mixture of particle sizes and densities. The model estimates the distribution of sediment particles transported as sand, silt, and clay, and the fraction of organic matter in the eroded sediment. SESOIL computations of sediment transport are performed for each particle size type, beginning at the upper end of a slope and routing sediment downslope.

The EROS model in SESOIL accounts for several surface features which may divert and slow the overland flow, allowing settling and deposition of the washload. These include vegetation, which slows the flow and filters out particles, and topography, which includes surface characteristics such as roughness and the existence of small depressions. Change in slope and loss of water through infiltration into the soil will reduce the flow rate and encourage settling of soil particles. Organic matter is distributed among the particle types based on the proportion of primary clay in each type (Foster et al., 1980). Soil receiving the deposited sediment is referred to as enriched. EROS computes sediment enrichment based on the ratio of the surface area of the sediment and organic matter to that of the surface area of the residual soil (Knisel et al., 1983).

3.4.1 Implementation In SESOIL

The EROS model uses characteristic rainfall and runoff factors for a storm to compute erosion and sediment transport for that storm (Foster et al., 1980). Hydrologic input to the erosion component consists of rainfall volume, rainfall erosivity, runoff volume, and the peak rate of runoff for each storm event. These terms drive soil detachment and subsequent transport by overland flow. Note that input data for the hydrologic cycle of SESOIL include total monthly precipitation, the number of storms per month, and the mean time of each rainfall event. Since SESOIL provides only monthly estimates of hydrologic parameters and in order to couple the SESOIL and EROS models, a statistical method is used to generate the amount of rainfall and duration of each storm for every rainfall event during the month. This algorithm employs a model featuring probability distributions in order to estimate the individual storm parameters (Eagleson, 1978; Grayman and Eagleson, 1969).

The washload cycle has been implemented with two subroutines in addition to the EROS, model PARAM and STORM, which take the input data for and results generated by the hydrologic cycle and adapt them for use. The PARAM subroutine supports EROS by first retrieving the hydrologic input data (e.g. the number of storm events per month and the depth of rainfall) read by SESOIL and then setting specific parameters applicable to the STORM and EROS subroutines. The STORM subroutine then uses the PARAM results and statistically generates information about each storm using the algorithm mentioned above. Thus, the coupled SESOIL/EROS model does not require any additional hydrologic input parameters for individual storms. However, it should be recognized that estimates of rainfall for each storm may be quite different than the actual values.

Additional data needed for the sediment cycle include the washload area, the fraction of sand, silt and clay in the soil, the average slope and slope length of the representative overland flow profile, the soil erodibility factor, the soil loss ratio, the contouring factor, and Manning's n coefficient for soil cover and surface roughness. Example values for these parameters can be found in the CREAMS documentation (Knisel, 1980; Foster et al., 1980). Note that the washload area should be less than or equal to the pollutant application area.

EROS takes the information generated by both the PARAM and STORM subroutines and computes estimates of the sediment yield for each month. Information from the sediment cycle, along with information from the hydrologic cycle, is then provided to the pollutant fate cycle, which will be discussed in the next subsection.

The coupled SESOIL/EROS model was evaluated by comparing predictions to published measured data (Hetrick and Travis, 1988). Two cornfield watersheds and one grassland watershed were included in the study. The sites differed in their management practices, soil type, ground cover, and meteorology. The model predictions were in fair to good agreement with observed data from the three watersheds, except for months where surface runoff came from one or two high intensity storms (Hetrick and Travis, 1988).

3.5 Pollutant Fate Cycle

The pollutant fate cycle focuses on the various chemical transport and transformation processes which may occur in the soil. These processes are summarized in Table 3.1, and are discussed in more detail in the subsections that follow. The pollutant fate cycle uses calculated results from the hydrologic cycle and the sediment washload cycle. Information from these cycles is automatically provided to the pollutant fate cycle.

In SESOIL, the ultimate fate and distribution of the pollutant is controlled by the processes interrelated by the mass balance equation (6) below. The processes are selectively employed and combined by the pollutant fate cycle based on the chemical properties and the simulation scenario specified by the user. The actual quantity or mass of pollutant taking part in any one process depends on the competition among all the processes for available pollutant mass. Pollutant availability for participation in these processes, and the pollutant rate of migration to the groundwater, depends on its partitioning in the soil between the gas (soil air), dissolved (soil moisture), and solid (adsorbed to soil) phases.

3.5.1 Foundation

In SESOIL, any layer (sublayer) can receive pollutant, store it, and export it to other subcompartments. Downward movement of pollutant occurs only with the soil moisture, while upward movement can occur only by vapor phase diffusion. Like the hydrologic cycle, the pollutant fate cycle is based on a mass balance

equation (Eq. 6) that tracks the pollutant as it moves in the soil moisture between subcompartments. Upon reaching and entering a layer or sublayer, the model assumes instantaneous uniform distribution of the pollutant throughout that layer or sublayer. The mass balance equation is:

$$O(t-1) + I(t) = T(t) + R(t) + M(t) \qquad (6)$$

where:

$O(t-1)$ = the amount of pollutant originally in the soil compartment at time t-1 ($\mu g/cm^2$),

$I(t)$ = the amount of pollutant entering the soil compartment during a time step ($\mu g/cm^2$),

$T(t)$ = the amount of pollutant transformed within the soil compartment during the time step ($\mu g/cm^2$),

$R(t)$ = the amount of pollutant remaining in the soil compartment at time t ($\mu g/cm^2$),

$M(t)$ = the amount of pollutant migrating out of the soil compartment during the time step ($\mu g/cm^2$).

The fate of the pollutant in the soil column includes both transport and transformation processes, which depend on the chemical's partitioning among the three phases: soil air, soil moisture, and soil solids. The three phases are assumed to be in equilibrium with each other at all times (see Diagram 2), and the partitioning is a function of user-supplied chemical-specific partition coefficients and rate constants. Once the concentration in one phase is known, the concentrations in the other phases can be calculated. The pollutant cycle of SESOIL is based on the chemical concentration in the soil water. That is, all the processes are written in terms of the pollutant concentration in soil water and the model iterates on the soil moisture concentration until the system defined by Eq. (6) balances.

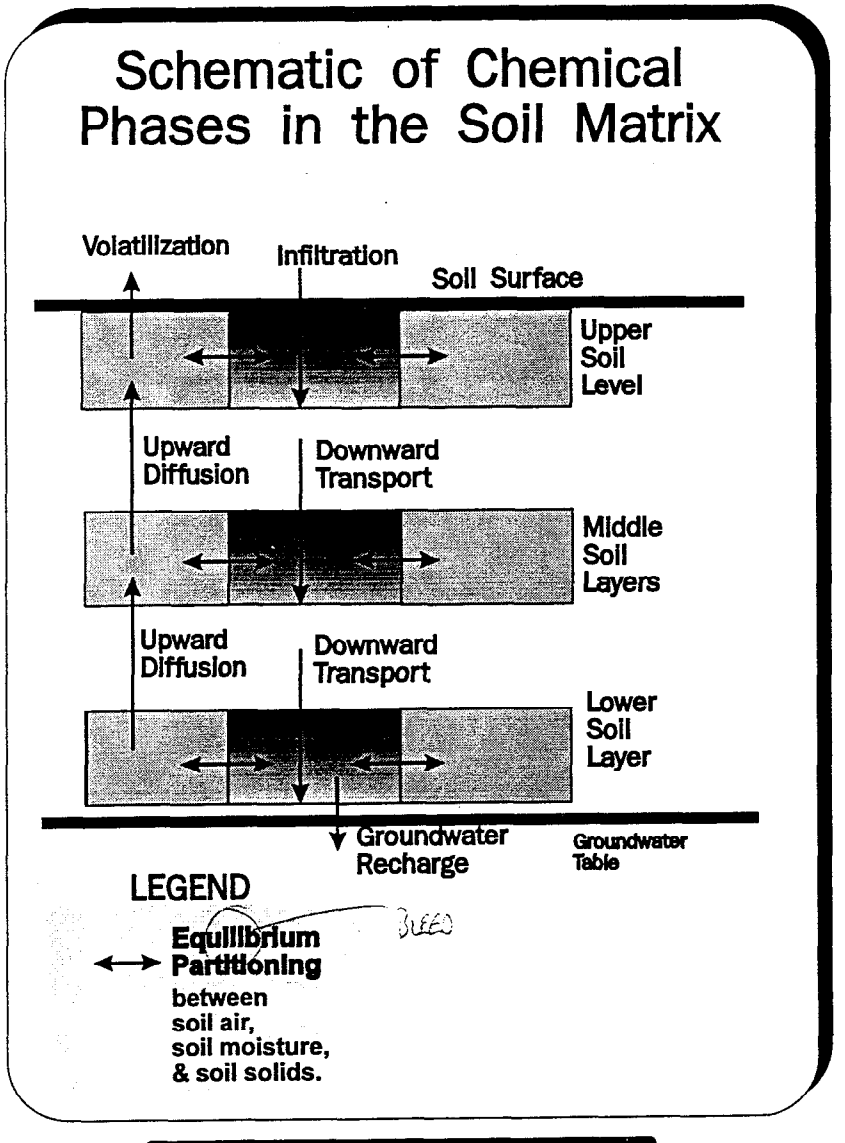
Schematic of Chemical Phases in the Soil Matrix
Volatilization
Infiltration
Soil Surface
Upper Soil Level
Upward Diffusion
Downward Transport
Middle Soil Layers
Upward Diffusion
Downward Transport
Lower Soil Layer
Groundwater Recharge
Groundwater Table
LEGEND
Equilibrium Partitioning between soil air, soil moisture, & soil solids.

DIAGRAM 2

The concentration in the soil air is calculated via the modified Henry's law:

$$c_{sa} = \frac{cH}{R(T+273)} \qquad (7)$$

where:

c_{sa} = pollutant concentration in soil air (µg/mL),

c = pollutant concentration in soil water (µg/mL),

H = Henry's law constant (m^3 atm/mol),

R = gas constant [$8.2*10^{-5}$ m^3atm/(mol ^oK)], and

T = soil temperature (^oC).

The concentration adsorbed to the soil is calculated using the Freundlich isotherm (note that a cation exchange option, discussed later, is available in SESOIL),

$$s = K_d c^{\frac{1}{n}} \qquad (8)$$

where:

s = pollutant adsorbed concentration (µg/g),

K_d = pollutant partitioning coefficient (µg/g)/(µg/mL),

c = pollutant concentration in soil water (µg/mL), and

n = Freundlich exponent.

The total concentration of the pollutant in the soil is computed as:

$$c_o = f_a \bullet c_{sa} + \theta \bullet c + \rho_b s \qquad (9)$$

where:

c_o = overall (total) pollutant concentration ($\mu g/cm^3$),

f_a = $f - \theta$ = the air-filled porosity (mL/mL),

f = soil porosity (mL/mL),

θ = soil water content (mL/mL), and

ρ_b = soil bulk density (g/cm^3).

In SESOIL, each soil layer (sublayer) has a set volume and the total soil column is treated as a series of interconnected layers. Each layer (sublayer) has its own mass balance equation [Eq. (6)] and can receive and release pollutant to and from adjacent layers (sublayers). Again, the individual fate processes that compose the SESOIL mass balance equations (e.g., volatilization, degradation) are functions of the pollutant concentration in the soil water of each zone and a variety of first-order rate constants, partitioning coefficients, and other constants. An iterative solution procedure is used to solve the system (the iteration parameter is **c**). See Bonazountas and Wagner (1984) for the numerical solution procedure.

The pollutant cycle equations are formulated on a monthly basis and results are given for each month simulated. However, to account for the dynamic processes in the model more accurately, an explicit time step of 1 day is used in the equations. The monthly output represents the summation of results from each day.

In the event that the dissolved concentration exceeds the aqueous solubility of the pollutant, the dissolved concentration is assumed to equal the aqueous solubility. That is, if during solution of the mass balance equation for any one layer, the dissolved concentration exceeds the solubility of the chemical, the iteration is stopped for that time step and the solubility is used as the dissolved concentration. The adsorbed and soil-air concentrations are calculated using the chemical partitioning equations as before [Eqs. (7) and (8)]. To maintain the mass balance, the remaining pollutant is assumed to remain in a pure phase (undissolved). Transport of the pure phase is not considered, but the mass of the chemical in the pure phase is used as input to that same layer in the next time step. Simulation continues until the pure phase eventually disappears. The pure

phase capability was not part of the original model and was added to SESOIL by Hetrick et al. (1989).

The discussion in the subsections that follow introduces the user to major algorithms and processes simulated in the pollutant cycle of SESOIL.

3.5.2 The Pollutant Depth Algorithm

The pollutant cycle in SESOIL is based on the pollutant concentration in soil moisture. In theory, a non-reactive dissolved pollutant originating in any unsaturated soil layer will travel to another soil layer or to the groundwater at the same speed as the moisture mass originating in the same soil layer. The movement of a reactive pollutant however, will be retarded in relation to the movement of the bulk moisture mass due to vapor phase partitioning and the adsorption of the pollutant on the soil particles. If it is assumed that no adsorption occurs, and the vapor phase is negligible, the pollutant will move at the same rate as water through the soil.

Originally, only the advective velocity was used in SESOIL to determine the depth the pollutant reached during a time step. The depth (D) was calculated as

$$D = \frac{J_w \, t_c}{\theta} \qquad (10)$$

where:

J_w = water velocity (cm/s),

t_c = advection time (s), and

θ = soil water content (cm^3/cm^3).

This approach allows all chemicals to reach the groundwater at the same time, irrespective of their chemical sorption characteristics. To account for retardation, SESOIL now uses the following equation to calculate the depth reached by a chemical with a linear equilibrium partitioning between its vapor, liquid, and adsorbed phases (Jury et al., 1984):

$$D = \frac{J_w t_c}{\theta + \rho_b K_d + \frac{f_a H}{R\,(T+273)}} \qquad (11)$$

SESOIL calculates the flux J_w for each layer using the infiltration rate and groundwater runoff (recharge) rate computed by the hydrologic cycle, and the depths and permeabilities input by the user. Note that a different permeability can be input for each of the four major soil layers. While the hydrologic cycle will use the weighted mean average of layer permeabilities according to Eq. (3), the pollutant cycle does take into account the separate permeability for each layer in computing J_w at the layer boundaries according to the following equation:

$$J_{w,z} = [G + (I - G)(\frac{d_j}{d})](\frac{k_i}{K_z}) \qquad (12)$$

where:

$J_{w,z}$ = infiltration rate at depth z, which will be the boundary between two major layers (cm/s),

G = groundwater runoff (recharge) (cm/s),

I = infiltration at surface (cm/s),

d_j = depth of soil column below depth z (cm),

d = depth of soil column from surface to groundwater table (cm),

K_z = intrinsic permeability defined by Eq. (3)cm^2), and

k_i = the vertically-averaged permeability for layer i (cm^2); is computed using Eq. (3) except d in the numerator of Eq. (3) is the sum of the layer depths above depth z and the summation in the denominator is from layer 1 to layer i.

The user is allowed two options for loading of pollutant: (1) a spill loading where all the pollutant is entered at the soil surface in the first time step of the month when the loading takes place, or (2) a steady application where the pollutant load is distributed evenly for each time step during the month at which the loading is specified. Option (1) allows loading at the soil surface only (layer 1, sublayer 1), whereas option (2) will allow loading in one or more of the four major layers. If sublayers are specified, the loading will always be entered into the first (top) sublayer of the major layer. Thus, while pollutant can be loaded in each of the four major layers, pollutant can not be loaded into each sublayer of a major layer to get a specific initial concentration distribution for the major layer.

☐ ***Side Note:*** *Although a spill loading can not be used in SESOIL for layers 2, 3, or 4, an initial soil-sorbed concentration can still be approximated for these layers. See Section 4.5 for more information and Appendix A contains an example.*

If there is a spill loading or if the pollutant is entered as a steady application in layer 1 (sublayer 1), then the depth of the pollutant front is calculated using Eq. (11) starting from the surface. If a steady loading is specified in layers 2, 3, and/or 4, then the depth of the pollutant front is assumed to begin at the **middle** of the lowest layer at which pollutant is loaded (sublayer 1 of that layer if sublayers are included) and Eq. (11) is used to compute the depth of the pollutant front from that point. Subsequently, the pollutant is not allowed to enter a layer/sublayer until the depth of the pollutant front has reached the top of that layer/sublayer. When the pollutant depth reaches the groundwater table, pollutant leaves the unsaturated zone by simply multiplying the groundwater runoff (recharge) rate by the concentration in the soil moisture.

3.5.3 Volatilization/Diffusion

In SESOIL, volatilization/diffusion includes movement of the pollutant from the soil surface to the atmosphere and from lower soil layers to upper ones. Note that vapor phase diffusion in SESOIL operates in the upward direction only. The rate of diffusion for a chemical is determined by the properties of the chemical, the soil properties, and environmental conditions. The volatilization/diffusion model in SESOIL is based on the model of Farmer et al. (1980) and Millington and Quirk (1961) and is a discretized version of Fick's first law over space, assuming vapor phase diffusion as the rate controlling process. That is, the same equation is used for volatilization to the atmosphere as is used for diffusion from lower layers to upper ones. The vapor phase diffusion flux through the soil J_a ($\mu g/cm^2 s$) is described as

$$J_a = -D_a \left(\frac{f_a^{\frac{10}{3}}}{f^2} \right) \frac{dC_{sa}}{dz} \qquad (13)$$

where:

D_a = the vapor diffusion coefficient of the compound in air (cm^2/s), and

C_{sa} = comes from Eq. (7) and **f** and $\mathbf{f_a}$ are as defined previously.

The volatilization algorithm in the original version of SESOIL allowed pollutant in the second (or lower) layer to volatilize directly to the atmosphere. This algorithm was modified by Hetrick et al. (1989). The pollutant can volatilize directly to the atmosphere from the surface layer, but if the chemical is in the second or lower layer, and the concentration in that layer is greater than the layer above it, then the chemical will diffuse into the upper layer rather than volatilize directly into the atmosphere.

An option the user has in the volatilization algorithm is to "turn off" the calculation by use of an input index parameter (for each layer). For example, if the index is set to 0.0 for each layer, the pollutant would not be allowed to diffuse upward or volatilize to the atmosphere; only downward movement of the pollutant with the soil moisture would occur. Also, if data are available, this index parameter can be varied to calibrate calculations to the measurements.

3.5.4 Sorption: Adsorption/Desorption And Cation Exchange

SESOIL includes two partitioning processes for movement of pollutant from soil moisture or soil air to soil solids. These are the sorption process and the cation exchange mechanism.

The sorption process may be defined as the adhesion of pollutant molecules or ions to the surface of soil solids. Most sorption processes are reversible, adsorption describing the movement of pollutant onto soil solids and desorption being the partitioning of the chemical from solid into the liquid or gas phase (Lyman et al., 1982). Adsorption and desorption are usually assumed to be occurring in equilibrium and are therefore modeled as a single process (Bonazountas et al., 1984). Adsorption is assumed to occur rapidly relative to the migration of the pollutant in soil moisture; it can drastically retard pollutant migration through the soil column.

SESOIL employs the general Freundlich equation (see Eq. 8 above) to model soil sorption processes. The equation correlates adsorbed concentration with the dissolved concentration of the pollutant, by means of an adsorption coefficient and the Freundlich parameter. This equation has been found to most nearly approximate the adsorption of many pollutants, especially organic chemicals, and a large amount of data have been generated and are available in the literature (see Bonazountas and Wagner, 1984; Fairbridge and Finke, 1979; Lyman et al., 1982).

For most organic chemicals, adsorption occurs mainly on the organic carbon particles within the soil (Lyman et al., 1982). The organic carbon partition coefficient (K_{oc}) for organic chemicals can be measured or estimated (Lyman et al., 1982). K_{oc} is converted to the partition coefficient (K_d) by multiplying by the fraction of organic carbon in the soil.

Values for the Freundlich exponent can be found in the literature. They generally range between 0.7 and 1.1, although values can be found as low as 0.3 and as high as 1.7. In the absence of data, a value of 1.0 is recommended since no estimation techniques for this parameter have yet been developed. Note that using 1.0 for the Freundlich exponent assumes a linear model for sorption (see Eq. 8).

The user is cautioned regarding indiscriminately using literature values for the partition coefficient K_d or the Freundlich exponent n, or estimation methods for K_d. There can be much variability in the values that are estimated or found in the literature compared to actual measurements for a site. For examples, refer to the study of Melancon et al. (1986).

Another option for modeling adsorption in SESOIL uses cation exchange capacity (CEC). Cation exchange occurs when positively charged atoms or molecules (cations such as heavy metals) are exchanged with the cations of minerals and other soil constituents. CEC is a measure amount of cations per unit of soil that are available for exchange with the pollutant.

The cation exchange algorithm in SESOIL is very simple and estimates the maximum amount of pollutant that can be adsorbed. The calculation of the pollutant immobilized by cation exchange is given by (from Bonazountas and Wagner, 1984):

$$MCEC = a \bullet CEC \bullet MWT / VAL \quad (14)$$

where:

$MCEC$	= maximum pollutant cation exchanged by the soil ($\mu g/g$ soil),
a	= 10.0 (units coefficient),
CEC	= cation exchange capacity of the soil (meq/100 g of dry wt. soil),
MWT	= molecular weight of the pollutant cation (g/mol),
VAL	= valence of the cation (-).

☐ ***Side Note:***
The cation exchange algorithm has been verified to be computationally correct in SESOIL, but it has not been validated with measured data.

With clays, the exchanged ion is often calcium, and clay soils tend to have the highest cation exchange capacity. Note that the CEC value of a soil increases with increase in pH, but pH is not included in the CEC algorithm in SESOIL. The CEC value must be adjusted manually to include effects due to pH.

In SESOIL, cation exchange computed by Eq. 14 is assumed to occur instantaneously, and irreversibly. Once maximum adsorption via exchange has been reached, no additional adsorption will be calculated. The process is also assumed to take precedence over all other soil processes in competition for the pollutant cation.

The use of the cation exchange subroutine is optional. If it is used, Eq. (8) should not be used (i.e., model inputs for K_d and K_{oc} should be 0.0) unless the user has selected the model inputs in such a way as to avoid double accounting. It is up to the user to be sure that cation exchange is the predominant adsorption mechanism at the modeled site. This determination includes considerations of leachate characteristics such as pH, ionic strength, and the presence and concentration of other cations. The other cations, often found in landfill leachate and aqueous industrial wastes, may have higher affinity for exchange with soil cations, and may effectively block exchange between the pollutant and the soil cations. In addition, the speciation of the pollutant should be considered (Bonazountas and Wagner, 1984).

3.5.5 Degradation: Biodegradation And Hydrolysis

The pollutant cycle of SESOIL contains two transformation routines which can be used to estimate pollutant degradation in the soil. Biodegradation is the biologic breakdown of organic chemicals, most often by microorganisms. Hydrolysis is a chemical reaction of the pollutant with water. Both processes result in the loss of

the original pollutant and the creation of new chemicals. The SESOIL model accounts for the mass of original pollutant lost via degradation but does not keep track of any degradation products. The user is responsible for knowing what the degradation products will be and their potential significance.

The biodegradation process is usually a significant loss mechanism in soil systems since soil environments have a diverse microbial population and a large variety of food sources and habitats (Hamaker,1972). Many environmental factors affect the rate of biodegradation in soil, including pH, moisture content of the soil, temperature, redox potential, availability of nutrients, oxygen content of the soil air, concentration of the chemical, presence of appropriate microorganisms, and presence of other compounds that may be preferred substrates. However, SESOIL doesn't consider these factors.

Biodegradation in SESOIL is handled as primary degradation, which is defined as any structural transformation in the parent compound which results in a change in the chemical's identity. It is estimated using the chemical's rate of decay in both the dissolved and adsorbed phases according to the first-order rate equation:

$$P_d = (C \bullet \theta \bullet k_{dl} + S \bullet \rho_b \bullet k_{ds}) \bullet A \bullet d_s \bullet \Delta t \qquad (15)$$

where:

P_d = decayed pollutant mass during time step Δt (μg),

k_{dl} = biodegradation rate of the compound in the liquid phase (day^{-1}),

k_{ds} = biodegradation rate of the compound in the solid phase (day^{-1}),

A = area of pollutant application (cm^2),

d_s = depth of the soil sublayer (cm),

Δt = time step (day), and

c, θ, s, and ρ_b are as defined for Eqs. (8) and (9).

Note that c, θ, and s are functions of time in the SESOIL model.

The use of a first-order rate equation is typical for fate and transport models and generally is an adequate representation of biodegradation for many chemicals. However, due to the many factors affecting biodegradation, in some cases a first-order rate may not be applicable to the site field conditions and a zero-order or a second- or higher-order rate might be more appropriate. The biodegradation algorithm in SESOIL that is described by Eq. (15) can not handle these cases.

The user is cautioned regarding the use of literature values for the biodegradation rates since these values are quite variable and in many cases are not applicable to site field conditions. In most cases, biodegradation rates are very site-specific and uncertainty in these rates must be recognized. The user-supplied first-order decay rate constants (for moisture and solids) should be values measured for the pollutant in a soil culture test under conditions similar to the site being modeled.

The SESOIL hydrolysis algorithm allows the simulation of neutral, acid- or base-catalyzed reactions and assumes that both dissolved and adsorbed pollutant are susceptible to hydrolysis (Lyman et al., 1982). Since hydrolysis is the reaction of the pollutant with water, this reaction may occur at any depth as the pollutant moves through the soil column. The hydrolysis subroutine requires user-supplied rate constants for the neutral, acid and base hydrolysis reactions of the pollutant, and the pH for each soil layer. The model does not correct for the temperature of the modeled soil.

☐ ***Side Note:***
The hydrolysis algorithm has been verified but has not been validated.

As for the biodegradation process, the algorithm for hydrolysis uses Eq. (15) except the rates k_{dl} and k_{ds} are both replaced by the rate constant k_h, defined as (from Bonazountas and Wagner, 1984):

$$k_h = k_o + k_H[H^+] + k_{OH}[OH^-] \qquad (16)$$

where:

k_h = the hydrolysis rate constant (day^{-1}),

k_o = rate constant for neutral hydrolysis (day^{-1}),

k_H = rate constant for acid-catalyzed hydrolysis ($days^{-1}mol^{-1}L$),

$[H^+]$ = 10^{-pH}, the hydrogen ion concentration (mol/L),

k_{OH} = rate constant for base-catalyzed hydrolysis ($days^{-1}mol^{-1}L$), and

$[OH^-]$ = 10^{pH-14}, the hydroxyl ion concentration (mol/L).

If cation exchange is considered, the following formula is used:

$$P_d = MCEC \bullet k_h \bullet \rho_b \bullet A \bullet d_s \bullet \Delta t \qquad (17)$$

where the parameters are as defined for Eqs. (9), (14), (15), and (16).

Extrapolating hydrolysis rates measured in a laboratory to the environment increases the uncertainty of model results if the hydrolysis rate is not corrected for the influences of temperature, adsorption, the soil ionic strength, and the possible catalytic effect of dissolved material or solid surfaces. Since there are usually large uncertainties in hydrolysis rates, the SESOIL model results for hydrolysis should be considered only as approximations. The rate of hydrolysis for various organic chemicals may vary over more than 14 orders of magnitude. In addition, the hydrolysis routine does not consider the influence of ionic strength or the presence of other dissolved organics on the hydrolysis rate of the pollutant.

☐ ***Side Note:***
The complexation routine has been verified but has not been validated.

3.5.6 Metal Complexation

Complexation, also called chelation, is defined here as a transformation process. In SESOIL, complexation incorporates the pollutant as part of a larger molecule and results in the binding of the pollutant to the soil. For example, metal cations (e.g. copper, lead, iron, zinc, cadmium) combine with organic or other nonmetallic molecules (ligands) to form stable complexes. The complex that is formed will generally prevent the metal from undergoing other reactions or interactions of the free ion.

The pollutant fate cycle incorporates a simplified representation of the complexation process as a removal process. It is only available for scenarios in which the pollutant is a heavy metal. The model assumes a reversible process in which a metal ion is complexed by a specified soluble organic ligand to form a complex which is soluble, non-adsorbable, and non-migrating. Possible ligands are humic acid, fulvic acid, and low molecular weight carboxylic acids, which are commonly found in landfill leachate (Bonazountas and Wagner, 1984) . It is the responsibility of the user to determine whether this process is likely to occur in the scenario being modeled, and to supply the appropriate information.

The complexation subroutine employs a nonlinear equation which must be solved numerically. It uses the same iterative procedure as the general pollutant cycle for monthly simulations. Required data include the stability (or dissociation) constant for the specific complex, and the mole ratio of ligand to metal. Also required are the molecular weights of the pollutant metal and the organic ligand. Equations used by this subroutine are based on the work of Giesy and Alberts (1984), Brinkman and Bellama (1978), and Sposito (1981). The model does not consider competition with metal ions in the soil which may have higher affinity for the ligand. Note that if the user chooses to model both cation exchange and metal complexation, the cation exchange process is assumed to occur first; ions involved in cation exchange are then unavailable for complexation. The general adsorption processes are modeled as being competitive with the complexation process (Bonazountas and Wagner, 1984).

3.5.7 Pollutant In Surface Runoff And Washload

Pollutant can be removed from the soil area being simulated by SESOIL via surface runoff and washload. The pollutant in surface runoff is simply the surface runoff computed in the hydrologic cycle (for each month) multiplied by the pollutant concentration in the soil moisture of the surface layer (for each time step). The result of this calculation is multiplied by another user-supplied parameter called ISRM, which controls the amount of chemical partitioned into runoff. There is no basis for estimating ISRM a priori; it can be set to 0.0 to "turn off" the pollutant participation in runoff, or it can be used essentially as a fitting parameter if data are available. In a calibration/validation exercise used to predict atrazine runoff at a site in Watkinsville, Georgia, the parameter ISRM was found to be 0.06 (see Hetrick et al., 1989).

Pollutant loss via washload is computed by taking the sediment yield from the washload cycle multiplied by the adsorbed pollutant concentration in the surface layer. While studies have been conducted comparing results of sediment yield with field data (Hetrick and Travis, 1988), pollutant loss via washload has not been validated in SESOIL.

3.5.8 Soil Temperature

The original SESOIL model assumed that soil temperature was equal to the user-supplied air temperature. The model was modified by Hetrick et al. (1989) to predict soil temperature from air temperature according to the following (Toy et al., 1978):

Summer: $Y = 16.115 + 0.856X$,
Fall: $Y = 1.578 + 1.023X$,
Winter: $Y = 15.322 + 0.656X$,
Spring: $Y = 0.179 + 1.052X$,
where:
Y = the mean monthly soil temperature (°F).
X = the mean monthly air temperature (°F).

These regression equations are very crude and not depth dependent. However, further complexity is not warranted since soil temperature is used only in Eq. (7) and does not significantly affect results. It should be noted that some chemical parameters and processes are dependent on temperature (for example, solubility,

Henry's law constant, and rate constants for biodegradation and hydrolysis). No explicit consideration of these effects is included in SESOIL, and the user should adjust the input values for such parameters if temperature effects are judged to be important.

3.5.9 Pollutant Cycle Evaluation

There are several approaches used to evaluate the reliability and usefulness of an environmental model, such as verification, calibration, sensitivity analysis, uncertainty analysis, and validation. Verification establishes that results from each of the algorithms of the model are correct. Calibration is the process of adjusting selected model parameters within an accepted range until the differences between model predictions and field observations are within selected criteria of performance (Donnigan and Dean, 1985). Sensitivity analysis focuses on the relative impact each parameter or term has on the model output, in order to determine the effect of data quality on output reliability. Uncertainty analysis seeks to quantify the uncertainty in the model output as a function of uncertainty in both model input and model operations. Validation also compares measured with predicted results, but includes analysis of the theoretical foundations of the model, focusing on the model's performance in simulating actual behavior of the chemical in the environment under study. (Note that the term validation has often been broadly used to mean a variety of things, including all five of the techniques mentioned above.)

A number of calibration, validation, and sensitivity studies have been performed on the SESOIL model. The model has been verified by extensive testing using extreme ranges of input data. Studies of the hydrologic and washload cycles have already been discussed above (see Sections 3.3 and 3.4). The following discusses the kinds of evaluations that have been performed on the pollutant cycle of the SESOIL model. Note that model validation is a continuing process; no model is ever completely validated.

To assess SESOIL's predictive capabilities for pollutant movement, a pollutant transport and validation study was performed by Arthur D. Little, Inc. under contract to EPA (Bonazountas et al., 1982). The application/validation study was conducted on two field sites, one in Kansas and one in Montana. SESOIL results were compared to data for the metals chromium, copper, nickel, and sodium at the Kansas site and the organics naphthalene and anthracene at the Montana site. Results showed reasonable agreement between predictions and measurements, although the concentrations of the metals were consistently underestimated, and the rate of metal movement at the Kansas site was consistently overestimated. At the Montana site, the concentrations of the organics were overestimated by SESOIL. Bonazountas et al. (1982) state that the overestimations for the organics were probably due to the fact that biodegradation was not considered in the simulations. Note that this study was done with the original SESOIL model, not the modified model that is described herein.

Hetrick et al. (1989) compared predictions of the improved version of SESOIL with empirical data from a laboratory study involving six organic chemicals (Melancon et al., 1986) and from three different field studies involving the application of aldicarb to two field plots (Hornsby et al., 1983; R. L. Jones, 1986; Jones et al., 1983, 1985) and atrazine to a single-field watershed (Smith et al., 1978). Results for several measures of pollutant transport were compared including the location of chemical peak vs. time, the time-dependent amount of pollutant leached to groundwater, the depth distribution of the pollutant at various times, the mass of the chemical degraded, and the amount of pollutant in surface runoff. This study showed that SESOIL predictions were in good agreement with observed data for both the laboratory study and the field studies.

SESOIL does a good job of predicting the leading edge of the chemical profile (Hetrick et al., 1989), due mainly to the improvement of the pollutant depth algorithm to include the chemical sorption characteristics (see Section 3.5.2 above). Also, when a split-sample calibration/validation procedure was used on 3 years of data from the single-field watershed, SESOIL did a good job of predicting the amount of chemical in the runoff. The model was less effective in predicting actual concentration profiles; the simulated concentrations near the soil surface underestimated the measurements in most cases. One explanation is that SESOIL does not consider the potential upward movement of the chemical with the upward movement of water due to soil evaporation losses.

SESOIL is a useful screening-level chemical migration and fate model. The model is relatively easy to use, the input data are straightforward to compile, and most of the model parameters can be readily estimated or obtained. Sensitivity analysis studies with SESOIL can be done efficiently. SESOIL can be applied to generic environmental scenarios for purposes of evaluating the general behavior of chemicals. Care should be taken when applying SESOIL to sites with large vertical variations in soil properties since the hydrologic cycle assumes a homogeneous soil profile. Only one value for the soil moisture content is computed for the entire soil column. If different permeabilities are input for each soil layer, the soil moisture content calculated in the hydrologic cycle using the vertically-averaged permeability (Eq. 3) may not be valid for the entire soil column. Thus, the user is warned that even though the model can accept different permeabilities for each layer, the effects of variable permeability are not fully accounted for by the model.

It is recommended that predictions for the hydrology at a given site be calibrated to agree with known measurements. Caution should be used when making conclusions based on modeling results when little hydrologic data exist against which to calibrate predictions. In these cases, it is recommended that the user employ sensitivity analysis or evaluate results obtained by assigning distributions to the input parameters (e.g., see Gardner, 1984; O'Neill et al., 1982; Hetrick et al., 1991). However, when properly used, SESOIL is an effective screening-level tool in assessing chemical movement in soils.

Building the SESOIL Model Inputs in RISKPRO

It is assumed that you have followed the installation guide for installing the RISKPRO system on your computer. Running the SESOIL model in RISKPRO is accomplished in two steps. First, the user creates the input files with the interface program built in RISKPRO called SEBUILD. Basically, this involves creating a series of files by retrieving data from the RISKPRO default menus, the chemical estimation programs, and/or entering information manually into the menu screens. Once the data have been input, the second step is to run the model. This is also done with the SEBUILD program, or at a later time by using the SERUN interface. SERUN requires the names of the input files you created in SEBUILD and then proceeds to read the information into the model and start the model run. The other computer capabilities from this menu are SEATLINK and SEGRAPH.

☐ ***Side Note:***
User should note that there is a stand alone FORTRAN code version of SESOIL that was developed to run both annual and monthly simulations. ***RISKPRO does not have the option of running an annual option.*** *SESOIL can be executed as a stand-alone program and the required input files can be assembled manually. The FORTRAN input format for these files can be found in Bonazountas and Wagner (1984).*

SEATLINK allows users to create input datasets for the groundwater model AT123D (Yeh, 1981) from the SESOIL output. These datasets include estimates of pollutant reaching the groundwater. The SEGRAPH program allows users to create graphs of model results by plotting one or more SESOIL output variables and will be discussed in Chapter 5.

The input data for the SESOIL model describe the physical or chemical characteristics of the model scenario. These input parameters can be determined or obtained independently either from lab analyses, field investigations, handbooks, or computer data bases. The RISKPRO system has automatic access to several datasets containing chemical, climate and soil information. SESOIL can execute various options depending on the available data and the objectives of the user's study. SESOIL will operate with data found or calculated in the RISKPRO chemical estimation program, other computer data bases, and/or handbooks.

Upon entering all information for the SEBUILD screens, the SEBUILD program stores the data into six output files which are later read by the SESOIL model. Each of these files (CLIMATE, SOIL, CHEM, APPLIC, WASH, and EXEC) are discussed below.

The input data files are created sequentially by the SEBUILD program. In general, for the creation of each file in RISKPRO, the SEBUILD program prompts the user to:

- ☐ **select the appropriate option for data entry (described below);**
- ☐ **enter, review, and/or modify the data file;**
- ☐ **provide data for the required number of years; and**
- ☐ **name the file.**

There are RISKPRO data bases available for each of the files, and an automatic access procedure is built into the SEBUILD program. The program also allows use of data in already existing files (e.g., files created from a previous SEBUILD run; with this option users can, for example, modify a few parameters at a time for a calibration or sensitivity run). SEBUILD allows the user to enter a number of years of data for each file. Alternatively, for a multiple year simulation, the user can supply a single year of data and the model will simply use that data for each of the subsequent years of the simulation. This option saves time and space by avoiding the entry of redundant data. This is also appropriate because the RISKPRO default climate data are long term average values. The SEBUILD menu allows the user to review and, if necessary, modify data to fit their specific scenario.

☐ ***Side Note:***
There are several options available for providing the data required by SESOIL. For each input file menu, there is a set of default data which has been collected based on recommendations from the SESOIL User's Guide (Bonazountas and Wagner,1984). Using default data may be appropriate if the site for the scenario is generic or if the data are not available in the appropriate RISKPRO data base or if site-specific data or literature values are not available.

4.1 Getting to the SESOIL Menu

☑ **Step 1** **Type RISKPRO at the DOS prompt and Figure 1 will appear.**

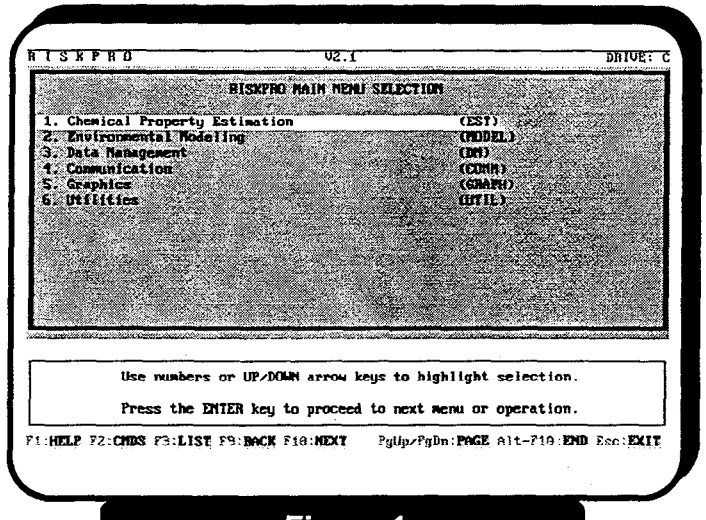
R I S K P R O
V2.1
DRIVE: C
RISKPRO MAIN MENU SELECTION
1. Chemical Property Estimation (EST)
2. Environmental Modeling (MODEL)
3. Data Management (DM)
4. Communication (COMM)
5. Graphics (GRAPH)
6. Utilities (UTIL)
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 1
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 1, choose the option 2, labeled *Environmental Modeling*, from the main selection menu and press the ENTER key.**

☑ **Step 3** **Choose option 3, labeled *Seasonal Soil Compartment Model*, as shown in Fig. 2 and press the ENTER key. You will find yourself at the Seasonal Soil Compartment Model Menu as shown in Fig. 3. The SEBUILD program option builds 5 input files: CLIMATE, SOIL, CHEM, APPLIC, and WASH. The WASH file is optional and needs to be created only if the washload simulation is to be performed. An additional input file, EXEC file, which contains SESOIL control parameters, is automatically created within the RISKPRO system by the SERUN program, and therefore you**

do not have to build this file. To start building your input files, choose option 1 from Fig. 3 (Build SESOIL input files). The first file that you build is the CLIMATE file, which is now discussed.

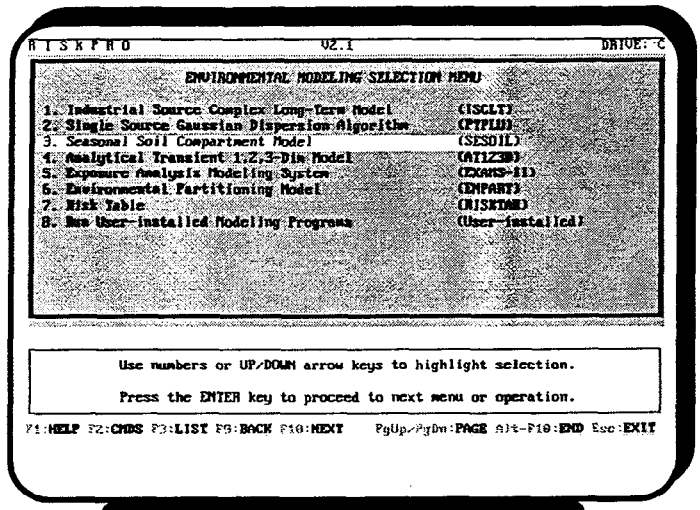
RISKPRO V2.1 DRIVE: C
ENVIRONMENTAL MODELING SELECTION MENU
1. Industrial Source Complex Long-Term Model (ISCLT)
2. Single Source Gaussian Dispersion Algorithm (PTPLU)
3. Seasonal Soil Compartment Model (SESOIL)
4. Analytical Transient 1,2,3-Dim Model (AT123D)
5. Exposure Analysis Modeling System (EXAMS-II)
6. Environmental Partitioning Model (EMPART)
7. Risk Table (RISKTAB)
8. Run User-installed Modeling Programs (User-installed)
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 2

Screen courtesy of General Sciences Corporation's RISKPRO™, Version 2.1© copyright 1991.

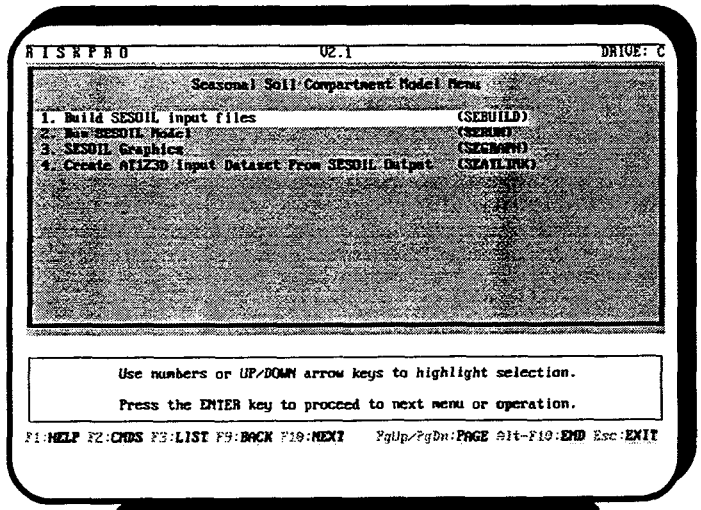
RISKPRO V2.1 DRIVE: C
Seasonal Soil Compartment Model Menu
1. Build SESOIL input files (SEBUILD)
2. Run SESOIL Model (SERUN)
3. SESOIL Graphics (SEGRAPH)
4. Create AT123D Input Dataset From SESOIL Output (SEATLINK)
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 3

Screen courtesy of General Sciences Corporation's RISKPRO™, Version 2.1© copyright 1991.

4.2 Building The CLIMATE Data File

☑ **Step 1** **Choose the SEBUILD option from the *Seasonal Soil Compartment Model Menu* (from Fig. 3). Figure 4 appears and shows the *CLIMATE Data Option* menu.**

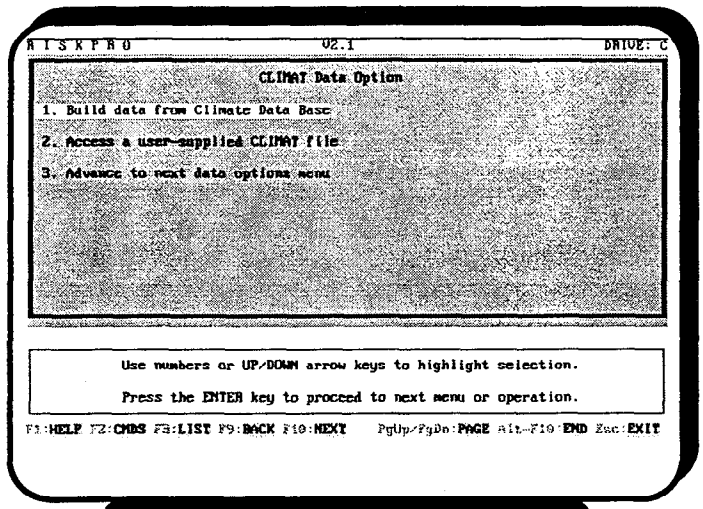
RISKPRO V2.1 DRIVE: C
CLIMAT Data Option
1. Build data from Climate Data Base
2. Access a user-supplied CLIMAT file
3. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 4
Screen courtesy of General Sciences Corporation's RISKPRO™, Version 2.1© copyright 1991.

☐ *OPTION 1* **as shown in Fig. 4, is labeled Build data from CLIMATE Data Base. This menu allows you to build the CLIMATE input file by selecting climate data from the Climate Data Base. You may then review and edit the data if desired. The data base in the RISKPRO system contains monthly average data for 262 first-order weather stations throughout the continental U.S. The data values for each month are based on monthly mean values for at least 10 years of observed data. See Section 4.2.1 below for more information.**

☐ *Side Note:*
A new Climate Data Base is available that contains 3162 weather stations.

☐ *OPTION 2* **as shown in Fig. 4, allows you to access a previously created CLIMATE data file. With this option a user may edit any climate data input parameter (see Section 4.2.2 below).**

☐ *OPTION 3* **as shown in Fig. 4, allows a user to advance to the next step of SEBUILD which would advance the user to building the SOIL data file (see Section 4.3 below).**

4.2.1 Creating The CLIMATE Data File From The Data Base

☑ **Step 1** Choose option one, labeled Build data from Climate Data Base, as shown in Fig. 4 and press the enter key. The next option, shown in Fig. 5, allows you to obtain a list of first-order climatic stations within a selected state. First-order stations have the most complete data gathering services. There are a total of 262 first-order stations located in or near 242 different cites throughout the US. This dataset was created in 1986 by the National Climatic Data Center of the National Oceanic and Atmospheric Administration.

☑ **Step 2** Enter either the state name, 2-letter state abbreviation, or 2-digit state FIPS code (for example for Wisconsin enter a 55 or WI) and advance to the next menu option by pressing the ENTER Key.

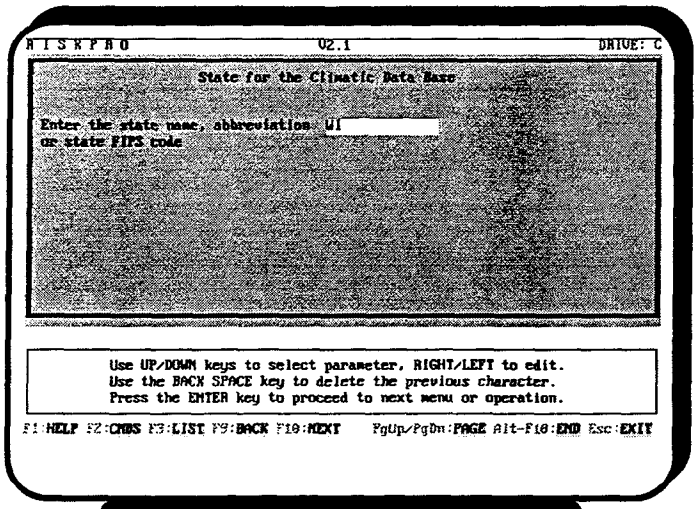
RISKPRO V2.1 DRIVE: C
State for the Climatic Data Base
Enter the state name, abbreviation, WI
or state FIPS code
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 5
Screen courtesy of General Sciences Corporation's RISKPRO™, Version 2.1™ copyright 1991.

☑ **Step 3** Next select the index of the desired station that you feel will represent the climatic condition for your site as shown in Fig. 6 and press the ENTER key to proceed to the next menu option. RISKPRO provides access to the Climate Data Base during the creation of this file, to provide measured values for a variety of climate properties.

☐ ***Side Note:***
The user should remember the latitude selected, as it will be required as a input parameter for the application data file.

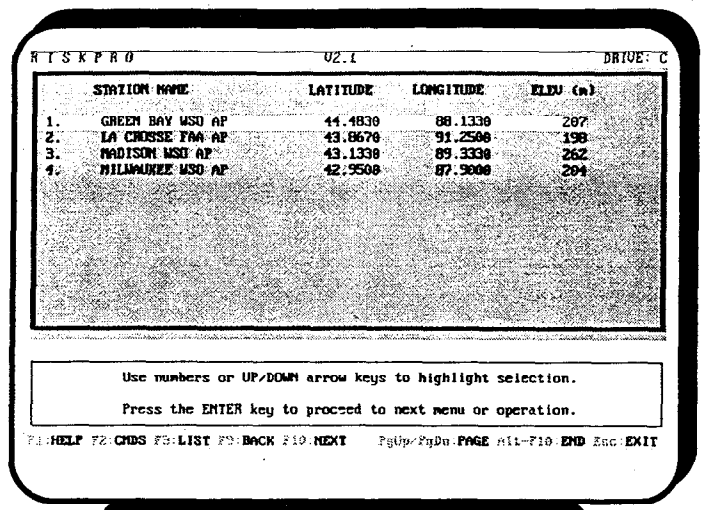
RISKPRO V2.1 DRIVE: C
STATION NAME LATITUDE LONGITUDE ELEV (m)
1. GREEN BAY WSO AP 44.4830 88.1330 207
2. LA CROSSE FAA AP 43.8670 91.2500 198
3. MADISON WSO AP 43.1330 89.3330 262
4. MILWAUKEE WSO AP 42.9500 87.9000 204
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 6
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 4** **As shown in Fig. 7, enter a descriptive label for the CLIMATE data file (up to 20 characters). This label appears in the catalog file of RISKPRO, and is used to identify the CLIMATE input file.**

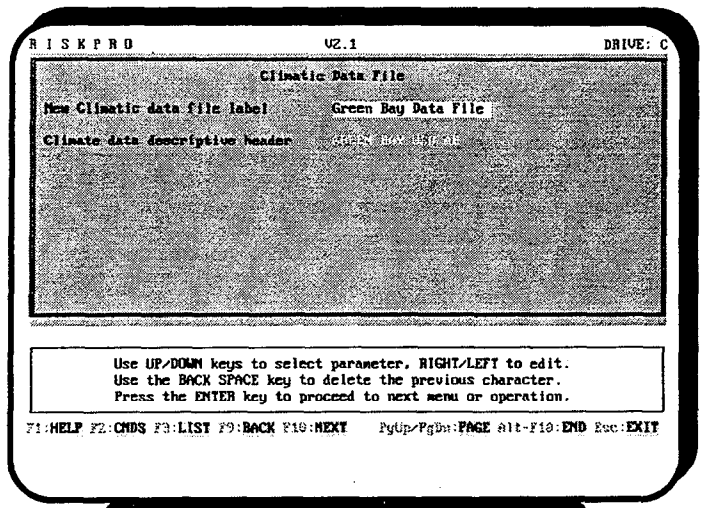
RISKPRO V2.1 DRIVE: C
Climatic Data File
New Climatic data file label Green Bay Data File
Climate data descriptive header
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 7
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 5** **Next use the down arrow key to select the option labeled *Climate data descriptive header* (see Fig. 8). Here enter a descriptive header for your CLIMATE data (up to 48 characters). This header appears in the SESOIL output file and is used to identify the input file. Press the ENTER key to proceed to the next menu.**

Your screen should now show you 4 options, as shown in Fig. 9, and has created one year of data where:

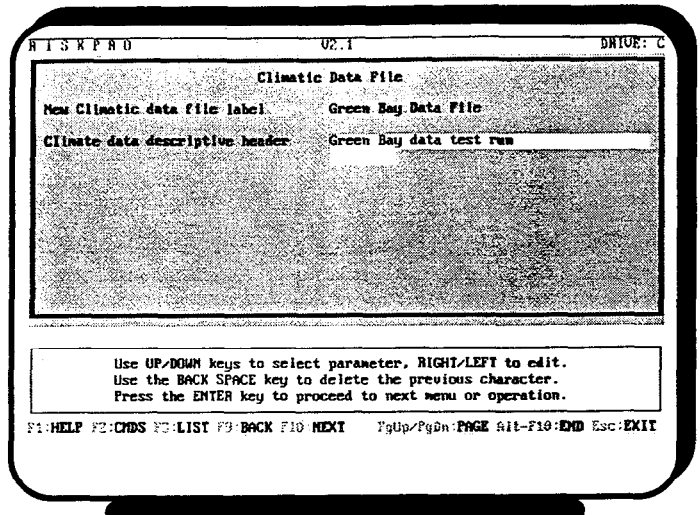
RISKPRO V2.1 DRIVE: C
Climatic Data File
New Climatic data file label: Green Bay Data File
Climate data descriptive header: Green Bay data test run
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 8
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

- ☐ ***OPTION 1*** labeled ***Edit an existing year of data*** allows you to review and modify any year of existing data.
- ☐ ***OPTION 2*** labeled ***Create additional years of data*** will allow you to create more years of data, using any of the existing years.
- ☐ ***OPTION 3*** labeled ***Delete existing years of data*** allows you to delete years of data already created.
- ☐ ***OPTION 4*** labeled ***Advance to the next data options menu*** in Fig. 9, allows you to proceed to the next menu once you have finished editing/creating your present monthly climatic data.

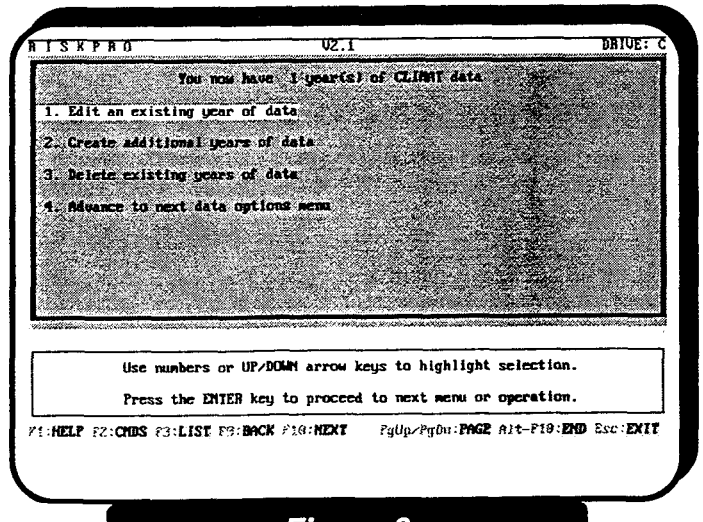
RISKPRO V2.1 DRIVE: C
You now have 1 year(s) of CLIMAT data
1. Edit an existing year of data
2. Create additional years of data
3. Delete existing years of data
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 9
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 6** **Next select the first option, labeled *Edit an existing year of data,* as shown in Fig. 9 and press the ENTER Key. With this selection you will see that RISKPRO has created one year of climatic data as shown in Fig. 10.**

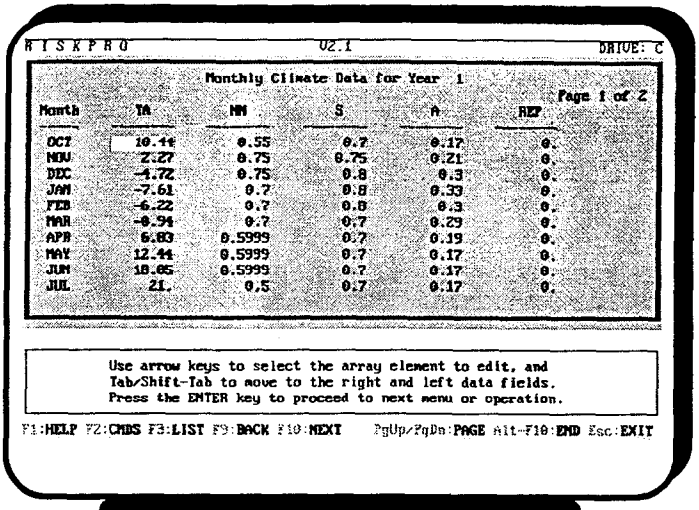
RISKPRO V2.1 DRIVE: C
Monthly Climate Data for Year 1
Page 1 of 2
Month TA NN S A REP
OCT 10.44 0.55 0.7 0.17 0.
NOV 2.27 0.75 0.75 0.21 0.
DEC -4.72 0.75 0.8 0.3 0.
JAN -7.61 0.7 0.8 0.33 0.
FEB -6.22 0.7 0.8 0.3 0.
MAR -0.94 0.7 0.7 0.29 0.
APR 6.83 0.5999 0.7 0.19 0.
MAY 12.44 0.5999 0.7 0.17 0.
JUN 18.05 0.5999 0.7 0.17 0.
JUL 21. 0.5 0.7 0.17 0.
Use arrow keys to select the array element to edit, and
Tab/Shift-Tab to move to the right and left data fields.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 10
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

This menu shows each of the CLIMATE data file array values that have been extracted from the RISKPRO database. These values are displayed in a tabular format starting with the month of October and ending with the month of September. The parameters shown in this menu are TA, NN, S, A, and REP where:

☐ *Side Note:*
When in the editing climate menu you can view and edit any of the climatic data values by using arrow keys to select the array element to edit, and Tab/Shift-Tab to move to the right and left data fields. Pressing the ENTER key will proceed you to the next menu

☒ *Parameter Description:*

TA = an array of the monthly mean air temperature for each month of the year (degrees Celsius), and is used in the estimation of evapotranspiration rates and soil temperatures. If the actual monthly evapotranspiration rates are known (i.e. non-zero values entered for REP), then TA is not used to calculate evapotranspiration. However, TA is always used to calculate soil temperature.

☒ *Parameter Description:*

NN= an array of the monthly mean cloud cover fraction for each month of the year (dimensionless fraction ranging from 0.0 to 1.0) used to calculate evapotranspiration rates. If the actual monthly evapotranspiration rates are known (i.e. non-zero values entered for REP) then NN in not used.

☒ *Parameter Description:* **S= an array of the monthly mean relative humidity for each month of the year (dimensionless fraction ranging from 0.0 to 1.0) used to calculate evapotranspiration rates. If the actual monthly evapotranspiration rates are known (i.e. non-zero values entered for REP), then S is not used.**

☒ *Parameter Description:* **A= an array of the short wave albedo fraction for each month of the year (dimensionless fraction ranging from 0.0 to 1.0) used to calculate evapotranspiration rates. If the actual monthly evapotranspiration rates are known (i.e. non-zero values entered for REP), then A is not used.**

☒ *Parameter Description:* **REP= an array of the monthly mean evapotranspiration rate (cm/day) for each month of the year. If zero is entered, SESOIL calculates evapotranspiration from TA, NN, S, and A. If a non-zero positive value is entered for REP, then it is used as the evapotranspiration rate, and TA, NN, S, and A are ignored for the evapotranspiration calculations.**

☑ **Step 7** **Next use your arrow keys to move up and down and Tab/Shift-Tab to move to the right and left to edit any array element. Remember to use your page down key to view and/or edit the months of August and September. Press the ENTER key to proceed to the next menu or operation.**

☑ **Step 8** **As shown in Fig. 11, the next menu selection is a continuation of the CLIMATE data file and includes the parameters MPM, MTR, MN, and MT, discussed below. Again, use your arrow keys to move up and down and Tab/Shift-Tab to move to the right and left to edit any array element. Remember also to use your page down key to view or edit the months of August and September. Press the ENTER key to proceed to the next menu.**

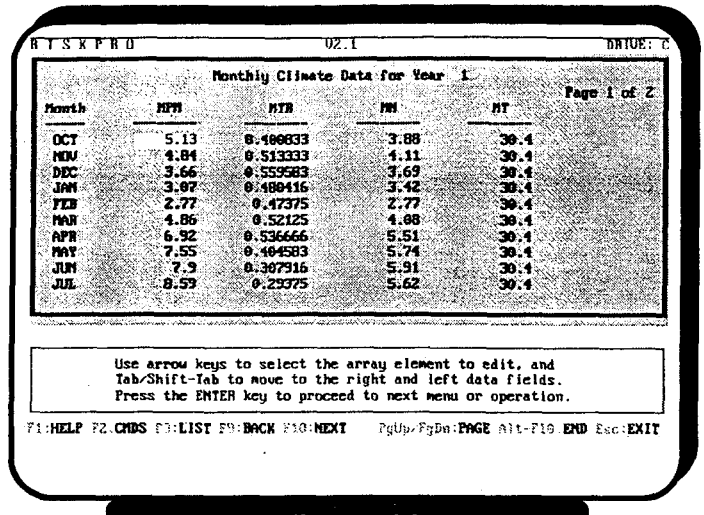
RISKPRO 02.1 DRIVE: C
Monthly Climate Data for Year 1
Page 1 of 2
Month MPM MTR MN MT
OCT 5.13 0.180833 3.88 30.4
NOV 4.84 0.513333 4.11 30.4
DEC 3.66 0.559583 3.69 30.4
JAN 3.07 0.480416 3.42 30.4
FEB 2.77 0.47375 2.77 30.4
MAR 4.86 0.52125 4.08 30.4
APR 6.92 0.536666 5.51 30.4
MAY 7.55 0.404583 5.74 30.4
JUN 7.9 0.307916 5.91 30.4
JUL 8.59 0.29375 5.62 30.4
Use arrow keys to select the array element to edit, and
Tab/Shift-Tab to move to the right and left data fields.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2.CHDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10 END Esc:EXIT

Figure 11
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☒ *Parameter Description:* **MPM=** an array of the total rain precipitation per month (cm/month).

☒ *Parameter Description:* **MTR=** an array of the mean duration of individual storm events (days) for each month of the year.

☒ *Parameter Description:* **MN=** an array of the number of storm events per month for each month of the year.

☒ *Parameter Description:* **MT=** an array of the length of the rainy season (days) for each month of the year. For most regions in the U.S., this parameter should be set to 30.4 (the default value) for all months, since rain events may occur throughout the entire month.

☑ **Step 9** Again, your screen should show that you now have 1 year of CLIMATE data (see Fig. 12) and you have the following four options, as shown in Fig. 12 where:

- ☐ *OPTION 1* allows you to review and modify any year of data that you have just created.
- ☐ *OPTION 2* allows you to create additional years of data, using any of the existing years that you have created. Remember that the total number of years of data you create does not necessarily have to equal the number of years you wish to simulate in your SESOIL run. If the number of years of available data is less than the number of years specified for the SESOIL run, the model

will automatically use the last year of available data for all remaining years of the simulation during the model run.

☐ *OPTION 3* **allows you to delete existing years of climate data. With this option you may delete existing years of data by entering the number of years to be deleted. The last N years of existing data will be deleted (i.e., entering "5" deletes the last 5 years of existing data.) You may not delete all years of data; i.e., data for year 1 must always exist.**

☐ *OPTION 4* **allows you to advance to the next menu option once you have finished editing/creating your present monthly data.**

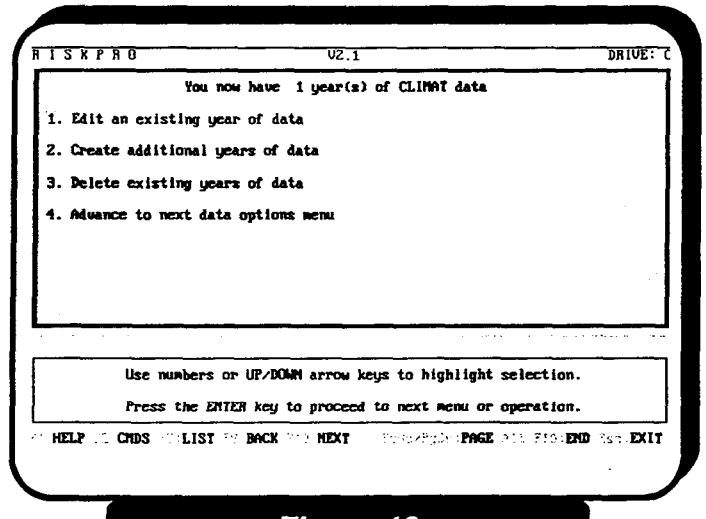
R I S K P R O
V2.1
DRIVE: C
You now have 1 year(s) of CLIMAT data
1. Edit an existing year of data
2. Create additional years of data
3. Delete existing years of data
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
HELP CMDS LIST BACK NEXT PAGE END EXIT

Figure 12
Screen courtesy of General Sciences Corporation's RISKPRO™, Version 2.1™ copyright 1991.

☑ **Step 10** **If you do not want to create or edit any more additional years of data choose option four, labeled *Advance to next data options menu (see Fig. 12).* Press ENTER to complete the building of your CLIMATE data file and proceed to the SOIL Data Options menu (Section 4.3). RISKPRO automatically creates the CLIMATE data file and inserts it in the catalog.**

4.2.2 Accessing A User-Supplied CLIMATE File

As shown in Fig. 13, choosing option 2, labeled *Access a user-supplied CLIMATE file*, allows you to access a previously created CLIMATE data file. You may modify the data as desired.

☑ **Step 1** **Choose option 2 as shown in Fig. 13 and press the ENTER key.**

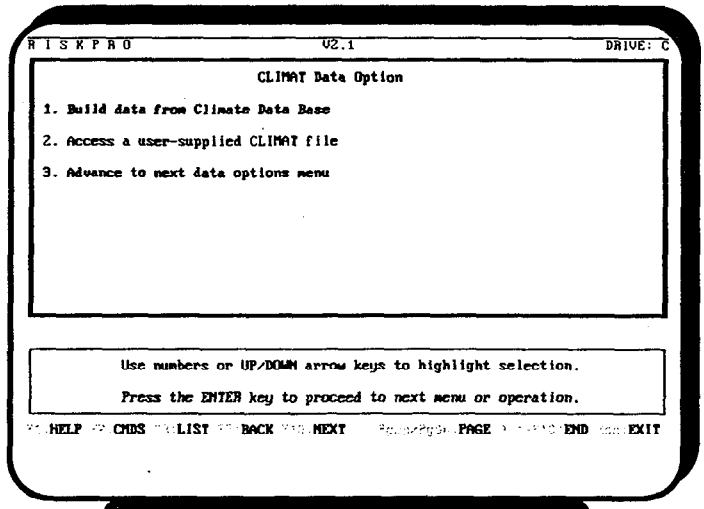
RISKPRO V2.1 DRIVE: C
CLIMAT Data Option
1. Build data from Climate Data Base
2. Access a user-supplied CLIMAT file
3. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
HELP CMDS LIST BACK NEXT PAGE END EXIT

Figure 13
Screen courtesy of General Sciences Corporation's RISKPRO©, Version 2.1© copyright 1991.

☑ **Step 2** **Next enter the file label name for your CLIMATE data file as shown in Fig. 14. If using a file previously created by RISKPRO, the file name is of the form SCLIMxxx.INP, where xxx are three digits. You may press the F3 function key for a list of files in your catalog (see Fig. 15). If no file extension is specified, then ".INP" will be assumed. Press ENTER to proceed to the next menu.**

☑ **Step 3** **Repeat steps 4-10 in Section 4.2.1 to edit your CLIMATE data file and to proceed to the SOIL data file (see Section 4.3).**

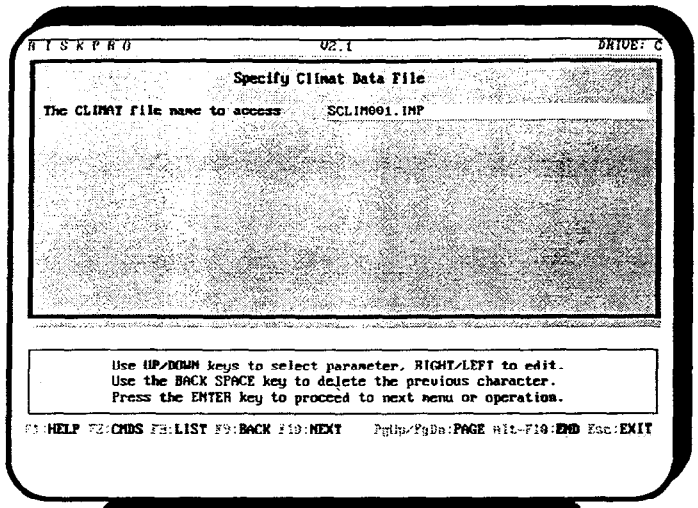
RISKPRO V2.1 DRIVE: C
Specify Climat Data File
The CLIMAT file name to access SCLIM001.IMP
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 14
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

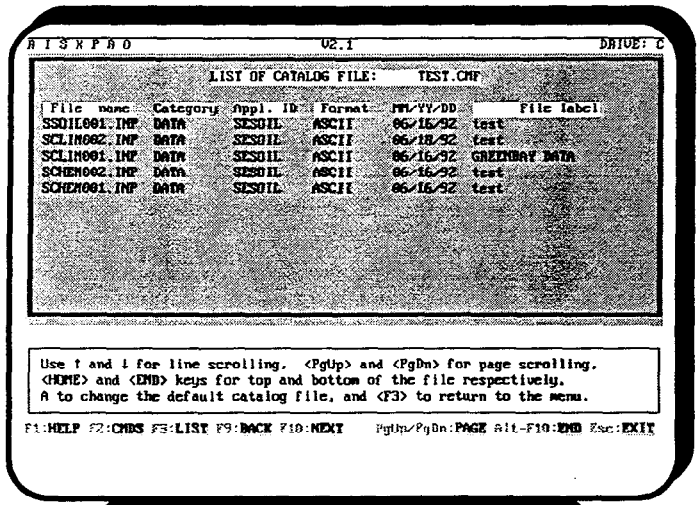
RISKPRO V2.1 DRIVE: C
LIST OF CATALOG FILE: TEST.CMF
File name Category Appl. ID Format MM/YY/DD File label
SSOIL001.IMP DATA SESOIL ASCII 06/16/92 test
SCLIM002.IMP DATA SESOIL ASCII 06/18/92 test
SCLIM001.IMP DATA SESOIL ASCII 06/16/92 GREENBAY DATA
SCHEM002.IMP DATA SESOIL ASCII 06/16/92 test
SCHEM001.IMP DATA SESOIL ASCII 06/16/92 test
Use ↑ and ↓ for line scrolling. <PgUp> and <PgDn> for page scrolling.
<HOME> and <END> keys for top and bottom of the file respectively.
A to change the default catalog file, and <F3> to return to the menu.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 15
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

4.2.3 Additional Information On The CLIMATE Data File

❑ ***Technical Note:*** *Model calculations determine the amount of precipitation which will enter the soil column (infiltration) and the amount which will become surface runoff. Water entering the soil column may either return to the atmosphere by the process of evapotranspiration and or migrate to the groundwater. Properties stored in the CLIMATE file are used by the model to simulate these processes. Air temperature, cloud cover, humidity, and albedo are automatically used to estimate evapotranspiration (REP), if a value for this parameter is not provided. If a value for REP is provided, the model will use that value and will not compute the estimate.*

4.3 Building the SOIL Data File

The next sequence of prompts and menus are for the creation of the SOIL file. This file is built by SEBUILD and contains information describing the properties of the soil profile. As shown in Fig. 16, there are three options from the main SOIL menu.

- ☐ *OPTION 1* **labeled *Select from a set of generic soils*, allows you to access soil data from a list of 14 generic soils and is discussed in Section 4.3.1. You may review and modify the data as desired.**
- ☐ *OPTION 2* **labeled *Access a user-supplied SOIL file*, allows you to access a previously created SOIL data file and is discussed in Section 4.3.2. You may modify the data as desired.**
- ☐ *OPTION 3* **labeled *Advance to next data options menu*, will advance you to the next menu to create the CHEM file and is described in Section 4.4.**

TABLE 4.1
SOIL DATA FILE PARAMETERS

Symbol	Parameter Description
SOIL NAME	Soil Name (0-48 char.)
RS	Bulk Density (g/cm^3)
K1	Intrinsic Permeability (cm^2)
C	Soil Disconnectedness Index (-)
N	Effective Porosity (-)
OC	Organic Carbon Content (%)
CEC	Cation Exchange Capacity (meq/100g)
FRN	Freundlich Exponent (-)

Table 4.1 describes each soil parameter. Further specific information for each input parameter is given in Section 4.3.3.

4.3.1 Creating A New SOIL File

☑ **Step 1** **To use one of the generic soil files in the RISKPRO system, first highlight option 1 as shown in Fig. 16 and press the EN-TER key. This selection will advance the user to the next menu.**

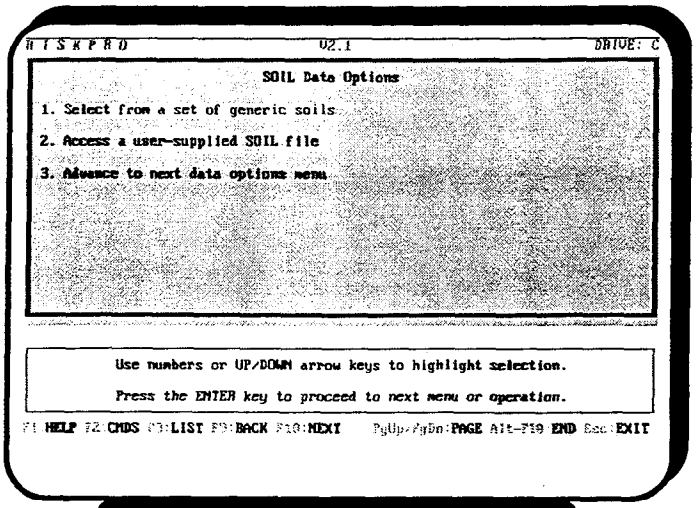
RISKPRO V2.1 DRIVE: C
SOIL Data Options
1. Select from a set of generic soils
2. Access a user-supplied SOIL file
3. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10 END Esc:EXIT

Figure 16
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 17, you can select soil data from a list of 14 generic soils within the RISKPRO system. Highlight the soil type of your choice, and press the ENTER key. Note that option 9 advances you to additional selections.**

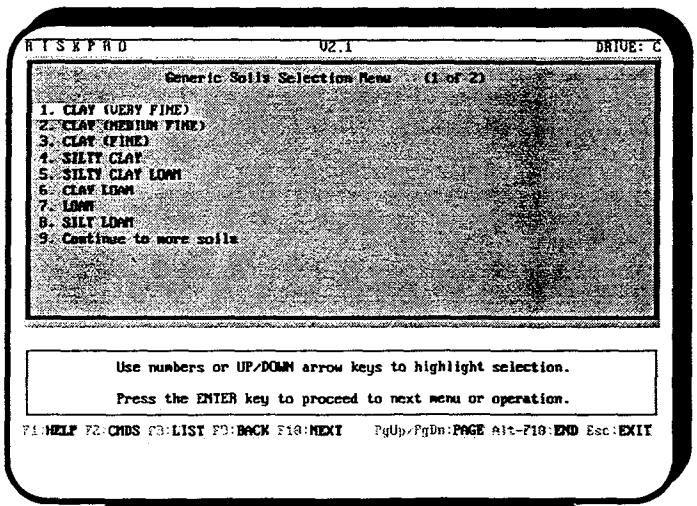
RISKPRO V2.1 DRIVE: C
Generic Soils Selection Menu (1 of 2)
1. CLAY (VERY FINE)
2. CLAY (MEDIUM FINE)
3. CLAY (FINE)
4. SILTY CLAY
5. SILTY CLAY LOAM
6. CLAY LOAM
7. LOAM
8. SILT LOAM
9. Continue to more soils
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 17
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ ***Side Note:***
The parameter K1 (overall soil intrinsic permeability) represents the average value for all the soil layers. K1 should be set to 0.0 if multiple K1's are used in the APPLIC file, described later.

☑ **Step 3** **Next you will be prompted to enter a descriptive label for the SOIL data file (up to 20 characters) as shown in Fig. 18. This label appears in the RISKPRO file catalog manager and is used to identify the soil input files.**

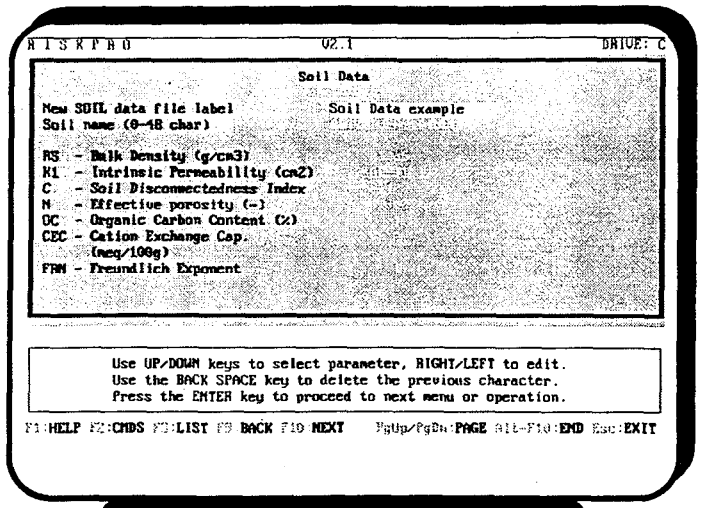
RISKPRO V2.1 DRIVE: C
Soil Data
New SOIL data file label
Soil name (0-48 char)
Soil Data example
BS - Bulk Density (g/cm3)
K1 - Intrinsic Permeability (cm2)
C - Soil Disconnectedness Index
N - Effective porosity (-)
OC - Organic Carbon Content (%)
CEC - Cation Exchange Cap. (meq/100g)
FRN - Freundlich Exponent
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9 BACK F10 NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 18
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 4** **Use the down arrow key to highlight the soil name. Enter a descriptive name for the SOIL data (up to 48 characters) as shown in Fig. 19. This header appears in the output report file. Note that when selecting a default soil this field is automatically filled. You may either change the name of the header file at this point or accept its default name by moving to the next field with the down arrow key.**

☐ ***Side Note:***
Additional soil properties for non-uniform soils are stored in the APPLIC file, described later.

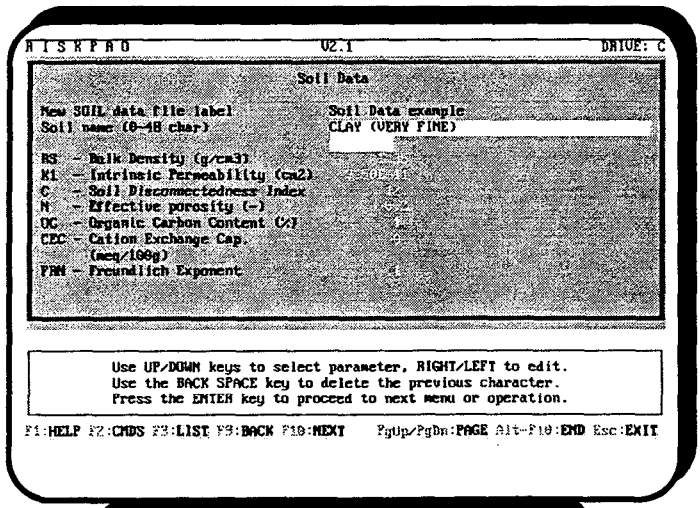
RISKPRO V2.1 DRIVE: C
Soil Data
New SOIL data file label
Soil name (0-48 char)
Soil Data example
CLAY (VERY FINE)
BS - Bulk Density (g/cm3)
K1 - Intrinsic Permeability (cm2)
C - Soil Disconnectedness Index
N - Effective porosity (-)
OC - Organic Carbon Content (%)
CEC - Cation Exchange Cap. (meq/100g)
FRN - Freundlich Exponent
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 19
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ ***Side Note:*** ***You*** *may enter your data in either scientific notation as shown in the default menu or in decimal format. RISKPRO will accept either format.*

☑ **Step 5** **Next you may either accept the default values of all the remaining soil parameters that are shown in Fig. 19 by pressing the ENTER key or enter new values by using the up/down arrow keys to highlight and edit each soil parameter field. When**

finished editing, press the ENTER key to proceed to the next menu (CHEM file, Section 4.4). RISKPRO will tell you the SOIL file was successfully inserted in the file catalog.

4.3.2 Accessing A User Supplied Data File

☑ Step 1 As shown in Fig. 20, highlight option 2 labeled *Access a user-supplied SOIL file* , and press the ENTER key. This option allows you to access a previously created SOIL data file. You may modify the data as desired.

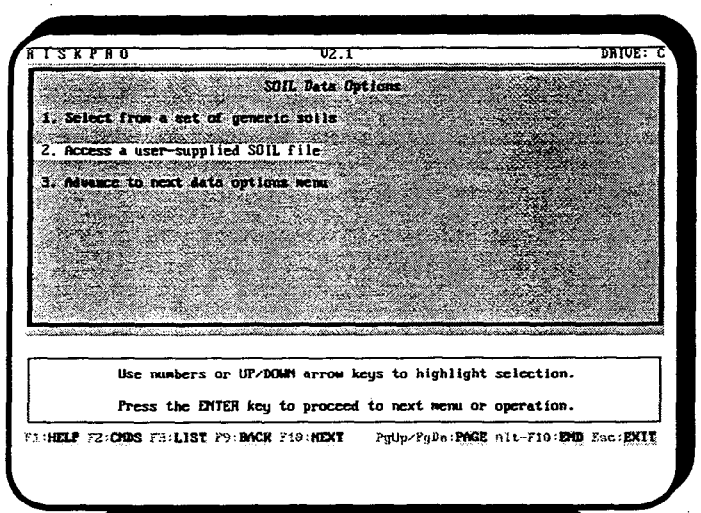
RISKPRO V2.1 DRIVE: C
SOIL Data Options
1. Select from a set of generic soils
2. Access a user-supplied SOIL file
3. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CHRS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 20

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☑ Step 2 Enter the file name for your SOIL data file as shown in figure Fig. 21 and press the ENTER key. Note that if no extension is specified, the extension ".INP" will be assumed. If using a file created by the RISKPRO system, the file name is of the form SSOILxxx.INP, where xxx are three digits. Remember that you may press the F3 function key for a list of files in your catalog.

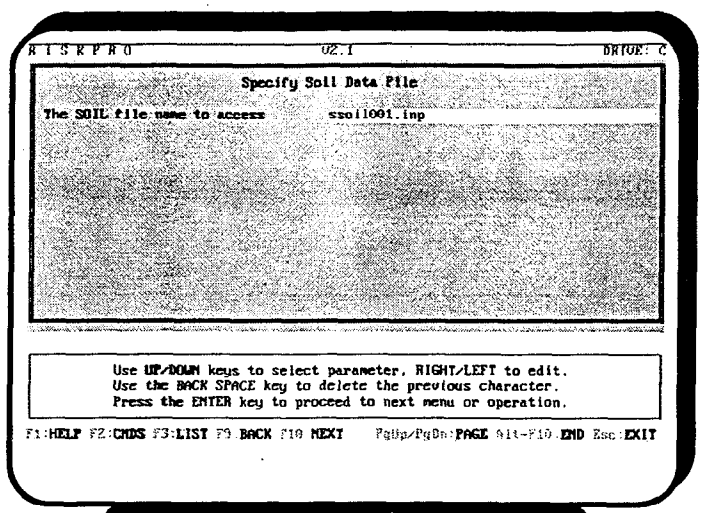
RISKPRO V2.1 DRIVE: C
Specify Soil Data File
The SOIL file name to access ssoil001.inp
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9 BACK F10 NEXT PgUp/PgDn:PAGE Alt-F10 END Esc:EXIT

Figure 21
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **Repeat steps 3 - 5 as described in Section 4.3.1 to complete building your data file and to proceed to the CHEM data menu.**

4.3.3 Additional Information On The SOIL Data Parameters

The following parameter descriptions and tables are provided as a guideline for each of the soil parameters used in SESOIL. The parameter definitions are also available from the RISKPRO system menu help screens. More details on these parameters are provided in Bonazountas and Wagner (1984).

☐ *Side Note:*
Intrinsic permeability, soil disconnectedness index, and effective porosity have been found to be sensitive parameters in SESOIL.
It is recommended these values be varied to calibrate results to field data at your site (see Section 3.3.3).

☒ *Parameter Description:* **RS= the average dry soil bulk density (g/cm^3) for the entire soil profile. See table 4.2 for typical values.**

☒ *Parameter Description:* **K1= the average soil intrinsic permeability (cm^2) for the entire soil profile. If K1 is 0, then the layer-specific intrinsic permeabilities (K11, K12, K13 and K14) specified in the APPLIC data file are used instead. Note: As an approximation, multiply hydraulic conductivity in units of cm/sec by 1.0E-5 to obtain intrinsic permeability, K1, in cm^2. Table 4.3 lists default values of K1 for SESOIL (Bonazountas and Wagner, 1984).**

☐ *Side Note:*
You can not enter a value less than 3.5 for C

☒ *Parameter Description:* **C= the soil pore disconnectedness index (unitless) for the entire soil profile. Its value typically ranges from 3.7 for sand to 12.0 for fine clay. It relates the soil permeability to the soil moisture content**

(see Section 3.3.3). See Table 4.4 for default values of C for SESOIL (Bonazountas and Wagner, 1984).

☒ *Parameter Description:* N= the effective porosity for the entire soil profile (unitless). N is defined by Eagleson (1978) as $N = (1-s_r)n_t$ where n_t is the porosity (volume of voids / total volume) and s_r is the residual medium saturation (volume of water unmoved by natural forces / volume of voids). N should generally have a value that is close to that for n_t and typically ranges from 0.2 to 0.4. See Table 4.5 for default values of N for SESOIL (Bonazountas and Wagner, 1984).

☒ *Parameter Description:* OC= the organic carbon content of the uppermost soil layer (%). The relative values of OC for the lower layers are specified in the APPLIC data file.

☒ *Parameter Description:* CEC= the cation exchange capacity (milliequivalents per 100 gram dry soil) of the uppermost soil layer. The relative values of CEC for the lower layers are specified in the APPLIC data file.

☒ *Parameter Description:* FRN= the Freundlich Equation Exponent used to determine chemical sorption for the top soil layer (see Eq. 8). The relative values of FRN for the lower layers are specified in the APPLIC data file. Values of FRN typically range from 0.9 to 1.4. If the value is not known, the default value of 1.0 is recommended.

Table 4.2
General ranges used for soil bulk density RS (g/cm^3)

Sand	*Silt*	*Clay*
1.18 - 1.58	1.29 - 1.80	1.40 - 2.20

TABLE 4.3
Default values of the intrinsic permeability, K1 (Bonazountas and Wagner, 1984)

USDA Textural Soil Class	K1 (cm^2)
Clay (very fine)	7.5E-11
Clay (medium fine)	2.5E-10
Clay (fine)	6.0E-10
Silty clay	5.0E-11
Silty clay loam	8.5E-11
Clay loam	6.5E-10
Loam	8.0E-10
Silt loam	3.5E-10
Silt	5.0E-11
Sandy clay	1.5E-9
Sandy clay loam	2.5E-9
Sandy loam	2.0E-9
Loamy sand	5.0E-8
Sand	1.0E-8

☐ ***Side Note:***
The default values for K1 may not be appropriate for a given soil or site. Use with care.

TABLE 4.4
Default values of the disconnectedness index C (Bonazountas and Wagner, 1984)

USDA Textural Soil Class	C
Clay (very fine)	12
Clay (medium fine)	12
Clay (fine)	12
Silty clay	12
Silty clay loam	10
Clay loam	7.5
Loam	6.5
Silt loam	5.5
Silt	12
Sandy clay	6
Sandy clay loam	4
Sandy loam	4
Loamy sand	3.9
Sand	3.7

❑ *Side Note:*
Although the values of N in Table 4.5 for clay type soils seem high, Bonazountas and Wagner (1984) found the values to be appropriate in their experience in using the SESOIL model. The authors concur with this experience; however, values of N in Table 4.5 should be used with care.

Table 4.5
Default values of the effective porosity, N (Bonazountas and Wagner, 1984)

USDA Textural Soil Class	N
Clay (very fine)	0.20
Clay (medium fine)	0.20
Clay (fine)	0.22
Silty clay	0.25
Silty clay loam	0.27
Clay loam	0.30
Loam	0.30
Silt loam	0.35
Silt	0.27
Sandy clay	0.24
Sandy clay loam	0.26
Sandy loam	0.25
Loamy sand	0.28
Sand	0.30

❑ ***Technical Note:*** *Values for bulk density, soil disconnectedness, and effective porosity are specified for the entire soil column. The intrinsic permeability can be specified for each layer in the APPLIC file discussed below (to do this, K1 in the soil file must be set to 0.0). Also, values for organic carbon content, the cation exchange capacity, and the Freundlich exponent may be varied down the soil profile by specifying ratios in the APPLIC file described below.*

❑ ***Technical Note:*** *If K11, K12, K13, and K14 are specified in the APPLIC file (see Section 4.5), an average value is calculated for the hydrologic cycle (see Eq. (3)). The separate values for each layer are used in the pollutant cycle (see Section 3.5.2).*

❑ ***Technical Note:*** *The bulk density, intrinsic permeability, and effective porosity are all interrelated parameters, yet only the intrinsic permeability can be varied from one layer to the next. Thus, if different K1's are used in the APPLIC file (discussed later), the bulk density and effective porosity may not be appropriate for the resultant permeability that is computed by Eq. (3).*

4.4 Creating the Chemical Data File

The next input file to be created by SEBUILD contains chemical property information for the chemical under study. Parameters used by the model are listed in Table 4.6. As shown in Fig. 22, there are several options offered by SEBUILD to enter chemical data.

- ☐ *OPTION 1* allows you to manually enter each of the chemical data values and is described in Section 4.4.1.
- ☐ *OPTION 2* allows access to chemical data from an AUTOEST output file and is described in Section 4.4.2. AUTOEST output files contain the chemical properties estimated by the AUTOEST chemical estimation program in RISKPRO. The values are automatically loaded into the SESOIL CHEM data menus. If you have purchased the chemical estimation program module, the RISKPRO system can provide you access to chemical estimation program output as input into the SESOIL CHEM files. This is useful when measured values for water solubility, the organic carbon partition coefficient, and the Henry's Law Constant are unavailable.
- ☐ *OPTION 3* provides access to the data from a previously created CHEM data file and is described in Section 4.4.3 . You may use the data as they are, or edit the data.
- ☐ *OPTION 4* advances to the next menu and is described in further detail in Section 4.5. It serves as an exit from the CHEM data options and advances you to the Application menu.

Table 4.6
Chemical Data

SYMBOL	PARAMETER DESCRIPTION
NAME	Chemical Name (0-48 char)
SL	Solubility in Water (µg/mL)
DA	Air Diffusion Coeff (cm^2/sec)
H	Henry's Law Const. (m^3-atm/mol)
KOC	OC Adsorption (µg/g oc)/(µg/mL)
K	Soil Adsorption (µg/g)/(µg/mL)
MWT	Molecular Weight (g/mole)
VAL	Valence (-)
KNH	Neutral Hydrolysis Const (1/day)
KBH	Base Hydrolysis Const (L/mol/day)
KAH	Acid Hydrolysis Const (L/mol/day)
KDEL	Liquid Phase Biodeg. Rate (1/day)
KDES	Solid Phase Biodeg. Rate (1/day)
SK	Ligand Stability Const (-)
B	Moles Ligand per Mole Compound(-)
MWTLIG	Molec. Wt. of Ligand (g/mol)

4.4.1 Entering Chemical Data Manually

☑ **Step 1** Choose the first option as shown in Fig. 22 and press the ENTER key to advance to the Chemical Data menu.

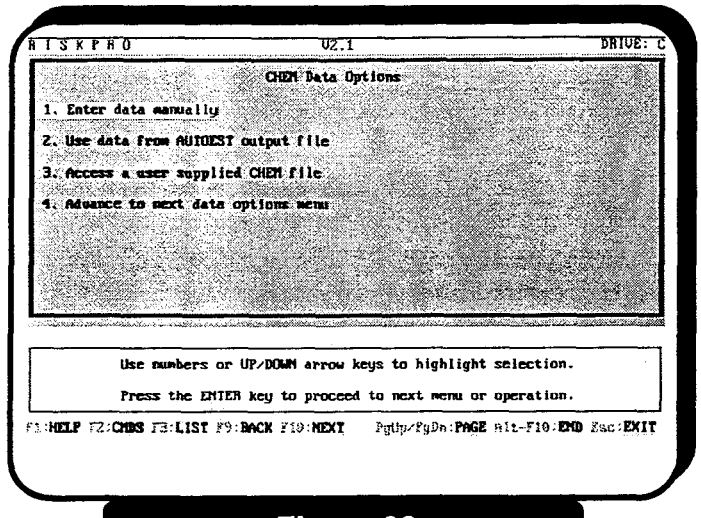
RISKPRO V2.1 DRIVE: C
CHEM Data Options
1. Enter data manually
2. Use data from AUTOEST output file
3. Access a user supplied CHEM file
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 22
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** As shown in Fig. 23 enter a descriptive label for the CHEMICAL data file (up to 20 characters). This label will appear in the file catalog manager and is used to identify the input CHEMICAL file.

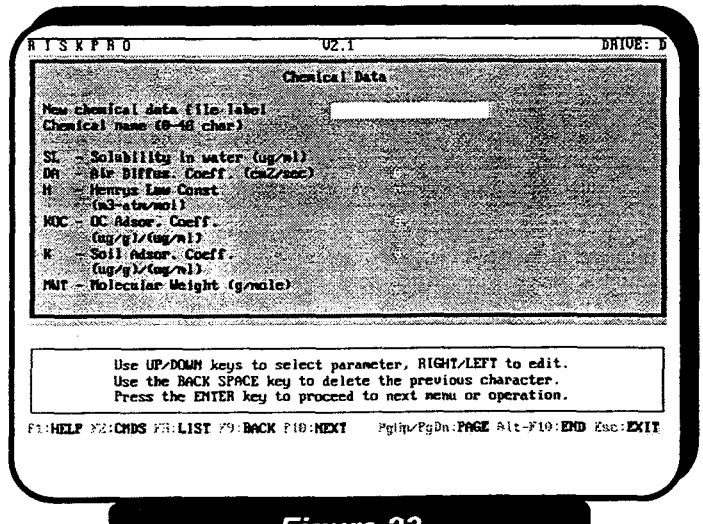
RISKPRO V2.1 DRIVE: D
Chemical Data
New chemical data file label
Chemical name (0-40 char)
SL - Solubility in water (ug/ml)
DA - Air Diffus. Coeff. (cm2/sec)
H - Henrys Law Const.
(m3-atm/mol)
KOC - OC Adsor. Coeff.
(ug/g)/(ug/ml)
K - Soil Adsor. Coeff.
(ug/g)/(ug/ml)
MWT - Molecular Weight (g/mole)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 23
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **Next use your down arrow key to highlight the CHEMICAL name as shown in Fig. 24. Enter the name of the chemical (up to 48 characters). This is a header which will appear in the output report file.**

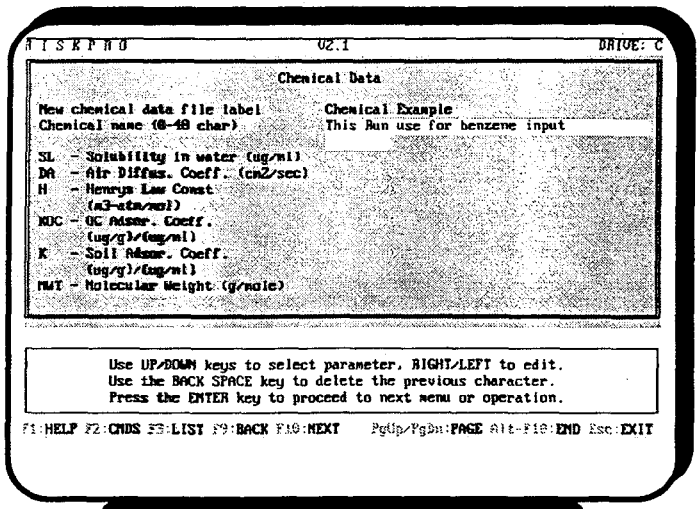
RISKPRO V2.1 DRIVE: C
Chemical Data
New chemical data file label Chemical Example
Chemical name (0-40 char) This Run use for benzene input
SL - Solubility in water (ug/ml)
DA - Air Diffus. Coeff. (cm2/sec)
H - Henrys Law Const (m3-atm/mol)
KOC - OC Adsor. Coeff. (ug/g)/(ug/ml)
K - Soil Adsor. Coeff. (ug/g)/(ug/ml)
MWT - Molecular Weight (g/mole)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 24
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ ***Side Note:***
Values entered in this file for KOC, K, KDEL, and KDES are assumed to be for the first soil layer and are used as a reference point for the other layers. The layer-specific ratios must be provided in the APPLIC file (see Section 4.5).

☑ **Step 4** **Next using the arrow keys, enter the values for SL, DA, H, KOC, K, and MWT (see parameter descriptions at the end of this section for more details or press the F1 key when highlighting each value).**

☑ **Step 5** **Next press the ENTER key to have the RISKPRO system accept your input values and to proceed *to the* More Chemical Data menu (see Fig. 25).**

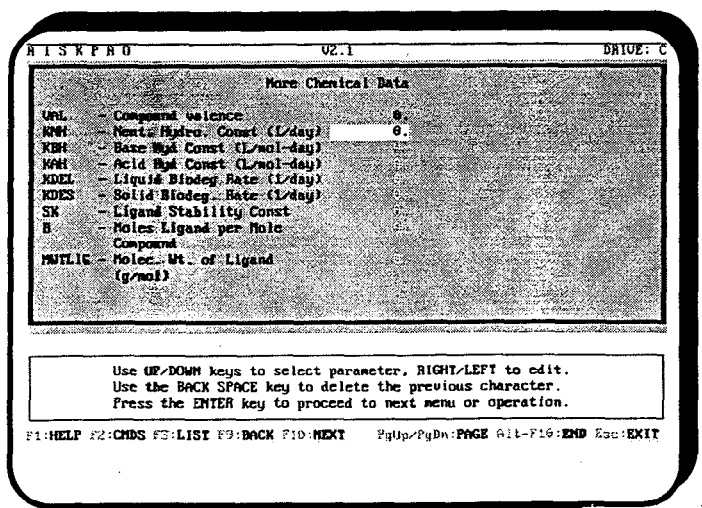
RISKPRO V2.1 DRIVE: C
More Chemical Data
VAL - Compound Valence 0.
KNH - Neut. Hydro. Const (L/day) 0.
KBH - Base Hyd Const (L/mol-day)
KAH - Acid Hyd Const (L/mol-day)
KDEL - Liquid Biodeg. Rate (1/day)
KDES - Solid Biodeg. Rate (1/day)
SK - Ligand Stability Const
B - Moles Ligand per Mole Compound
MWTLIG - Molec. Wt. of Ligand (g/mol)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 25
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 6** **Here you may either accept the default values of all the remaining chemical parameters that are shown in Fig. 25 by pressing the ENTER key or enter new values by using the up/down arrow keys. Press the ENTER key to proceed to the next menu (APPLIC File, Section 4.5). At this point you have built your CHEMICAL data file and RISKPRO will tell you the CHEMICAL file was successfully inserted in the file catalog.**

4.4.2 Entering Data From AUTOEST Output File Option

This option should be used to access the chemical data from an AUTOEST output file. AUTOEST output files contain the chemical properties estimated by the AUTOEST chemical estimation program in RISKPRO. The values are automatically loaded into the SESOIL CHEM data menus.

☑ **Step 1** **Choose the second option as shown in Fig. 26 and press the ENTER key to advance to the next menu.**

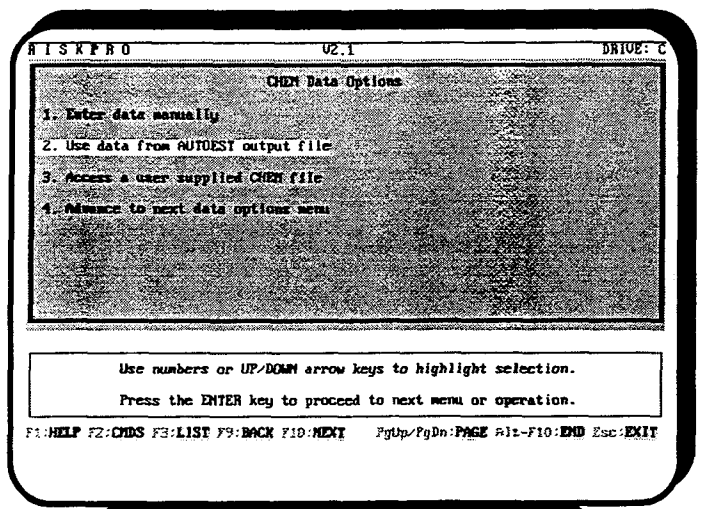
RISKPRO V2.1 DRIVE: C
CHEM Data Options
1. Enter data manually
2. Use data from AUTOEST output file
3. Access a user supplied CHEM file
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 26
Screen courtesy of General Sciences Corporation's RISKPRO™, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 27, enter the name of an output data file you have created with the AUTOEST program from the RISKPRO system and press the ENTER key. The file has a name in the form CHEMxxx.DAT, where xxx are three digits. Press the F3 function key to obtain a list of files in the file catalog.**

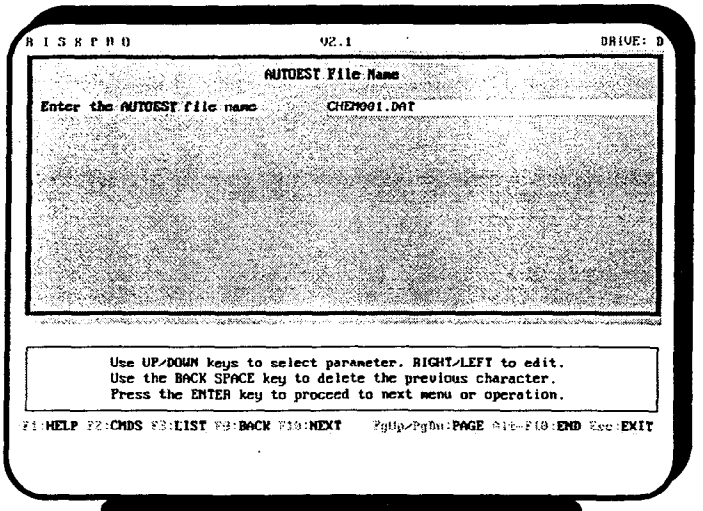
RISKPRO V2.1 DRIVE: D
AUTOEST File Name
Enter the AUTOEST file name CHEM001.DAT
Use UP/DOWN keys to select parameter. RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 27
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **As shown in Fig. 28 you will see an example of an output screen menu of chemicals that were created with the AUTOEST program. Note that each chemical is given an index number. After viewing this screen press ALT-F10 to be prompted to the next screen menu as shown in Fig. 29.**

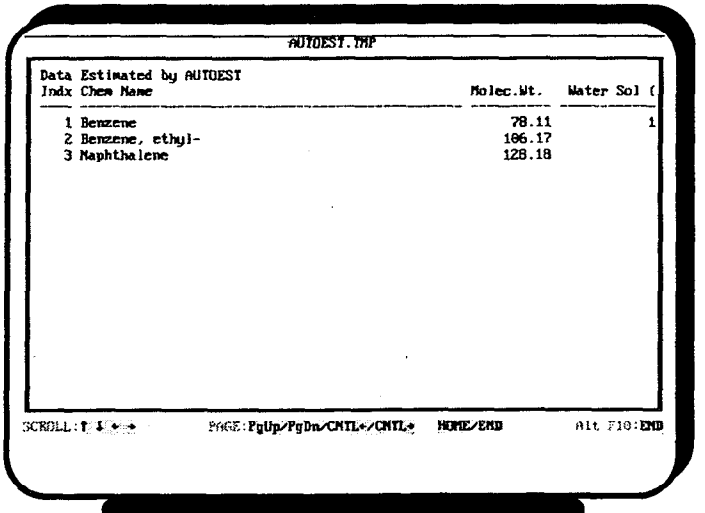
AUTOEST.TMP
Data Estimated by AUTOEST
Indx Chem Name Molec.Wt. Water Sol (
1 Benzene 78.11 1
2 Benzene, ethyl- 106.17
3 Naphthalene 128.18
SCROLL: PAGE:PgUp/PgDn/CNTL+/CNTL+ HOME/END Alt F10:END

Figure 28
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 4** **As shown in Fig. 29, enter the selected index number of the desired chemical and press the ENTER key.**

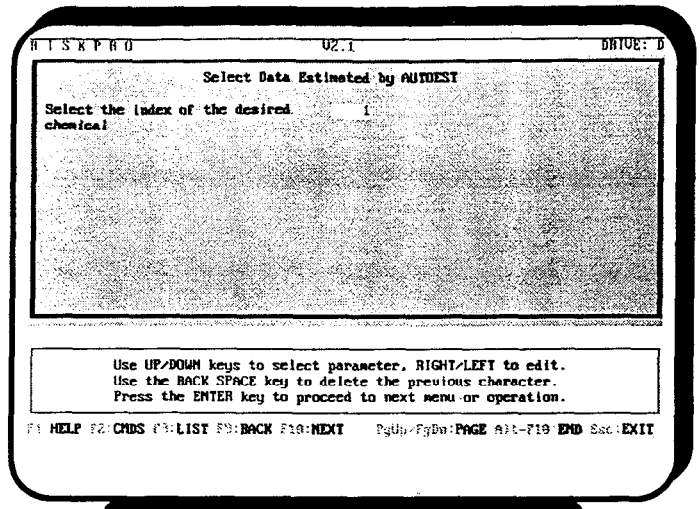
R I S K P R O
V2.1
DRIVE: D
Select Data Estimated by AUTOEST
Select the index of the desired chemical
1
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 29
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 5** **As you will notice in Fig. 30, the Chemical Data menu fields are automatically filled from the index number you entered. Repeat steps 2-6 as described in Section 4.4.1 and then proceed to the APPLIC menu.**

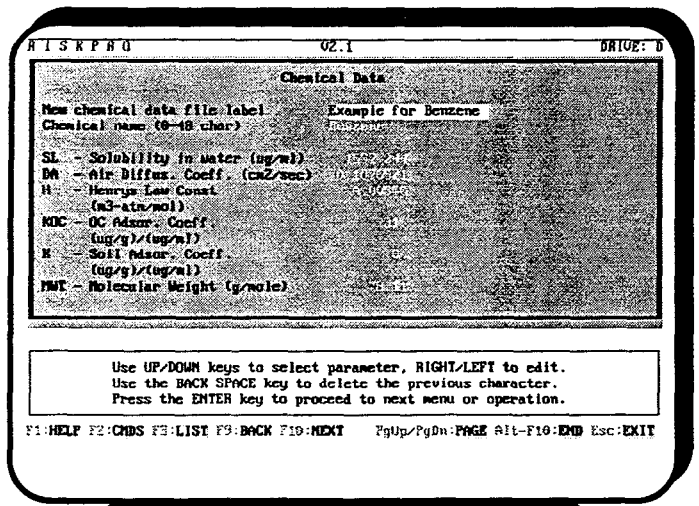
R I S K P R O
V2.1
DRIVE: D
Chemical Data
New chemical data file label
Example for Benzene
Chemical name (0-18 char)
SL - Solubility in water (ug/ml)
DM - Air Diffus. Coeff. (cm2/sec)
H - Henrys Law Const. (m3-atm/mol)
KOC - OC Adsor. Coeff. (ug/g)/(ug/ml)
K - Soil Adsor. Coeff. (ug/g)/(ug/ml)
MWT - Molecular Weight (g/mole)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 30
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

4.4.3 Accessing A User-Supplied CHEM File Option Menu

This option should be used to access the data from a previously created CHEM data file. You may use the data as they are, or edit the data.

☑ **Step 1** **Choose the third option as shown in Fig. 31 and press the ENTER key to advance to the next menu.**

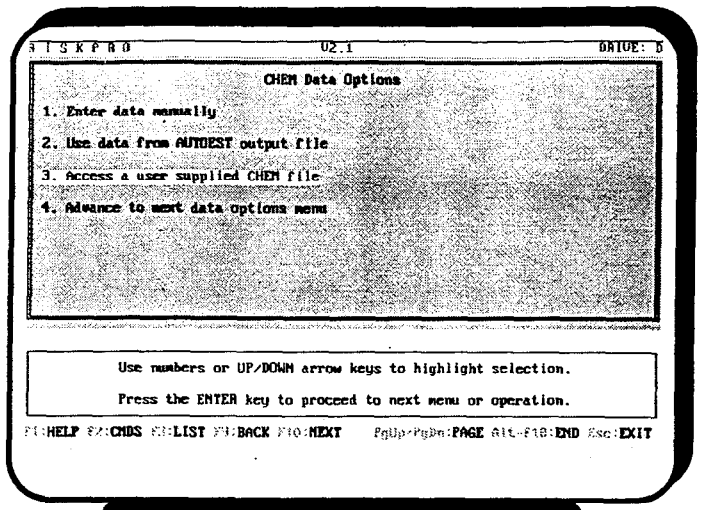
RISKPRO V2.1 DRIVE: D
CHEM Data Options
1. Enter data manually
2. Use data from AUTODEST output file
3. Access a user supplied CHEM file
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 31
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 32 enter the file name of your CHEMICAL data file and press the ENTER key. Again, if no extension is specified, the extension ".INP" will be assumed. If using a file previously created by RISKPRO, the file name is of the form SCHEMxxx.INP, where xxx are three digits. You may press the F3 function key for a list of files in your catalog.**

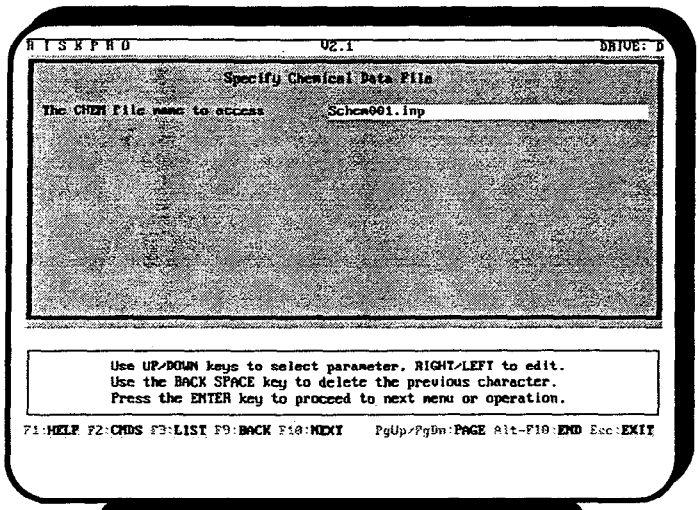
RISKPRO V2.1 DRIVE: D
Specify Chemical Data File
The CHEM file name to access Schem001.inp
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 32
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **Repeat steps 2-6 as described in Section 4.4.1 and then proceed to the APPLIC menu.**

4.4.4 Additional Information On The Chemical Data Parameters

☐ *Side Note:*
SESOIL requires a water solubility value for the chemical. If the water solubility is unknown and migration to groundwater is the concern, then an estimate that is somewhat high should be used. This will ensure that the estimates of chemical

The following notes are provided to help you better understand each of the chemical parameters use in the SESOIL CHEM data files and are also available from the RISKPRO system menu help screens.

☒ ***Parameter Description:*** **SL= the solubility of the compound in water (µg/mL or mg/L).**

☒ ***Parameter Description:*** **DA= the diffusion coefficient in air (cm^2/s), used to calculate volatilization. If the chemical data is accessed from an AUTOEST data file, then DA is estimated by the following relationship: DA = DA' * (MWT'/MWT)**0.5 where DA' is the known diffusion coefficient for a reference compound, MWT' is the molecular weight of the reference compound, and MWT is the molecular weight of the current compound. Trichloroethylene (TCE) is used as the reference compound having a diffusion coefficient of 0.083 cm^2/sec and a molecular weight of 131.5 g/mole.**

☐ *Side Note:*
MWT is used only if the complexation or cation exchange algorithms are used.

☒ ***Parameter Description:*** **H= dimensional form of Henry's Law constant (m^3-atm/mole), used in Eqs. (7), (11), and (13).**

☒ ***Parameter Description:*** **KOC= the adsorption coefficient of the compound on organic carbon (µg/g-OC)/(µg/mL). If the adsorption coefficient on the soil, K, is used, then enter zero for KOC, since KOC will not be used.**

☒ ***Parameter Description:*** **K= the adsorption coefficient of the compound on soil (µg/g)/(µg/mL). If a non-zero value is entered for K, SESOIL will use this value as the adsorption coefficient. Otherwise, KOC and OC (soil organic carbon content) will be used to calculate K as described in Section 3.5.4.**

☐ *Side Note:*
VAL is used only if the cation exchange algorithm is used.

☒ ***Parameter Description:*** **MWT= the molecular weight of the compound (g/mole).**

☒ ***Parameter Description:*** **VAL= the valence of the compound used to calculate cation exchange with soil. A positive integer number should be entered without a sign.**

☒ *Parameter Description:* **KNH= the neutral hydrolysis rate constant (L/mol/day).**

☒ *Parameter Description:* **KBH= the base hydrolysis rate constant (L/mol/day).**

☒ *Parameter Description:* **KAH= the acid hydrolysis rate constant (1/day).**

☒ *Parameter Description:* **KDEL= the biodegradation rate of the compound in the liquid phase (1/day).**

☐ *Side Note:* *SK, B, and MWTLIG are used only if the complexation algorithm is used.*

☒ *Parameter Description:* **KDES= the biodegradation rate of the compound in the solid phase (1/day).**

☒ *Parameter Description:* **SK= the stability (dissociation) constant of the compound/ligand complex. Zero should be entered if a ligand compound is not used.**

☒ *Parameter Description:* **B= the number of moles of ligand per mole of compound complexed. Zero should be entered if a ligand compound is not used.**

☒ *Parameter Description:* **MWTLIG= the molecular weight of the ligand (g/mole). Zero should be entered if a ligand compound is not used.**

☐ ***Technical Note:*** *Adsorption in SESOIL can be represented either by the overall partitioning coefficient K, which is often labeled Kd in the literature, or by the organic carbon:water partitioning coefficient, KOC. If a value for the overall adsorption coefficient is unknown, this parameter value should be entered as zero. In this case, SESOIL uses the product of KOC and the organic carbon fraction to produce an estimated value for K. If the user enters a measured value for K, the program will not perform the estimation. Values entered here for K and KOC are entered for the first soil layer and layer-specified ratios are provided in the APPLIC file.*

☐ ***Technical Note:*** *Additional processes for handling the binding of pollutant to soil constituents are included in the cation exchange and complexation options. The molecular weight and valence of the pollutant are used in cation exchange calculations. Complexation estimation requires the pollutant's molecular weight, the molecular weight of the ligand participating in the complex, the moles of ligand per mole of pollutant in the complex, and the stability constant of the pollutant/ligand complex.*

☐ ***Technical Note:*** *Cation exchange and complexation are primarily used for metals and values for the parameters can be set to zero for most other applications.*

4.5 Creating The APPLIC File

The fourth file created in this process holds the information describing the specifics of the chemical release or application to the soil column. This information includes the dimensions of the soil column, the definition of soil layers (e.g., depths), and several additional soil properties beyond those specified in the soil (e.g., pH). Vertical variation of soil properties for nonuniform soils consisting of 2, 3, or 4 layers may also be described in this file. This variation is represented by assuming that the information supplied in the SOIL and CHEM files apply to the uppermost layer.

There are several options available for obtaining or entering the required data.

- **The first option allows you to access general APPLIC default data (see Section 4.5.1).**
- **The second option allows you to access default data for a generic municipal landfill. You may edit the default values to create your desired APPLIC data (see Section 4.5.2).**
- **The third option accesses a previously created APPLIC file. You may use the data as they are, or you may edit the data (see Section 4.5.3).**
- **The final option will advance you to the next menu. This option serves as an exit from building the APPLIC data file .**

For any of these options, the user can tailor the data for a particular scenario. Several years of data may be entered into the soil column or the user may provide one year of data and specify that this year of data is to be used for all remaining years of the simulation. Table 4.7 shows general information required for the application site.

Table 4.7
General Application Data

SYMBOL	PARAMETER DESCRIPTION
HEADER	Applic. Area Name (0-48 char)
ILYS	Number of Soil Layers
AR	Application Area (cm^2)
LAT	Latitude of Site (deg N)
ISPILL	Spill index (0 or 1)

4.5.1 Entering Application Data (General Data)

☑ **Step 1** Choose the first option as shown in Fig. 33 and press the ENTER key to advance to the next menu.

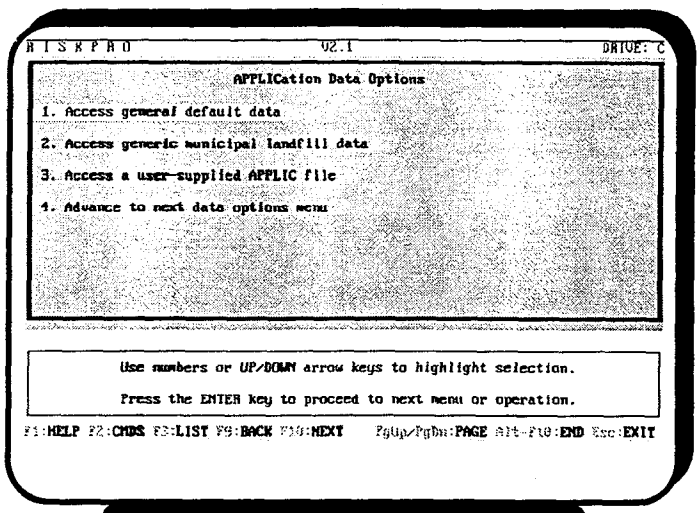
RISKPRO V2.1 DRIVE: C
APPLICation Data Options
1. Access general default data
2. Access generic municipal landfill data
3. Access a user-supplied APPLIC file
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 33
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** As shown in Fig. 34, enter a descriptive label for the APPLICATION data file (1 to 20 characters). This label appears in the file catalog manager and is used to identify the file.

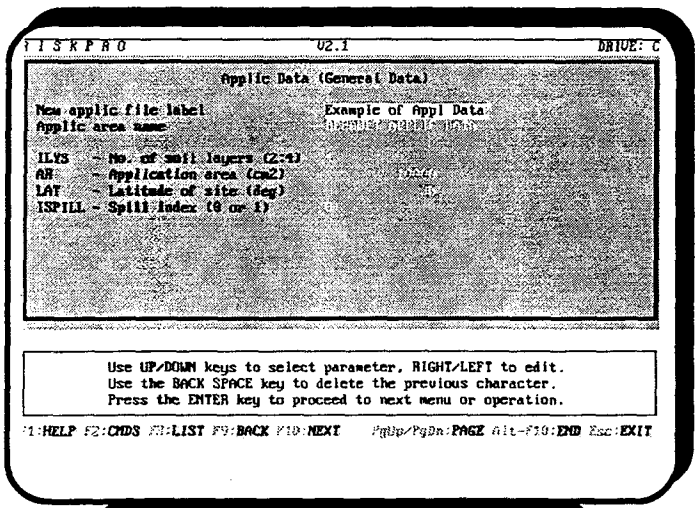
RISKPRO V2.1 DRIVE: C
Applic Data (General Data)
New applic file label
Applic area name
Example of Appl Data
ILYS - No. of soil layers (2:4)
AH - Application area (cm2)
LAT - Latitude of site (deg)
ISPILL - Spill Index (0 or 1)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 34
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☑ **Step 3** As shown in Fig. 35 use the down arrow key to highlight the descriptive header field and enter a description for your application site (0-48 characters). This header appears in the output report file.

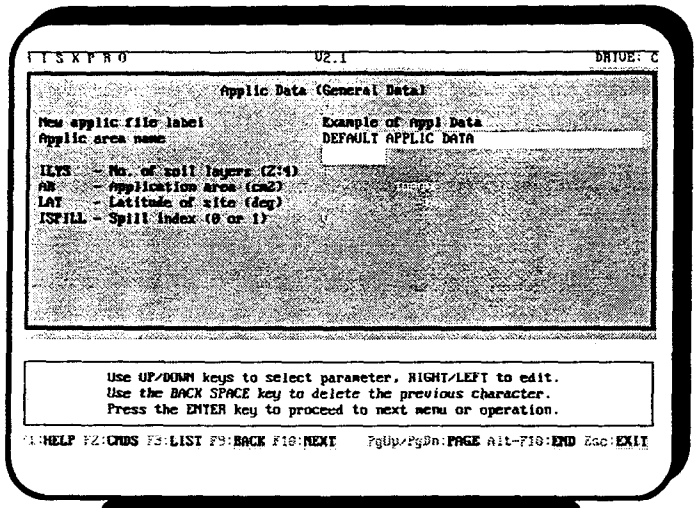
RISKPRO V2.1 DRIVE: C
Applic Data (General Data)
New applic file label
Applic area name
Example of Appl Data
DEFAULT APPLIC DATA
ILYS - No. of soil layers (2:4)
AR - Application area (cm2)
LAT - Latitude of site (deg)
ISPILL - Spill index (0 or 1)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F5:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 35
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☑ **Step 4** **Next highlight the ILYS option using your down arrow key . Enter the number of soil layers (zones) in the soil profile. The minimum number of layers required is 2, and the maximum is 4. Note that the default value is 4.**

☑ **Step 5** **Highlight the AR field. Enter the area of the application in cm^2. This is the top area of the soil compartment. Note the default value is 10000 cm^2. The actual area of application is important only when mass flux is considered. Concentration values are unaffected by area because it is constant for all layers.**

☑ **Step 6** **Next highlight the LAT field. Enter the latitude in decimal degrees . The latitude of the application site should correspond with the location of your climate data site since it is used along with the CLIMATE file parameters TA, S, A and NN for calculation of evapotranspiration.**

☐ *Side Note:*
ISPILL =1 applies only to the first layer (see Section 3.5.2).

☑ **Step 7** **Highlight the ISPILL field. ISPILL is an index indicating if the application loadings are instantaneous spills (pulses) or continuous loadings. Set ISPILL to 1 for instantaneous spill(s) occurring at the beginning of the month or set ISPILL to 0 for a continuous loading rate occurring throughout the month.**

☑ **Step 8** **If all your data for this menu are correct press the ENTER key to have RISKPRO accept your input values and to proceed to the APPLIC Data (Layer Specific Data) menu.**

☑ **Step 9** **As shown in Fig. 36, you have the option of entering the thickness of each layer (D1 through D4) in centimeters and the number of sublayers for each layer NSUB1 through NSUB4, by highlighting each field. Note that:**

☒ *Parameter Description:* **D1= thickness of the uppermost soil layer (cm).**

☒ *Parameter Description:* **D2= thickness of the second soil layer (cm).**

☒ *Parameter Description:* **D3= thickness of the third soil layer (cm).**

☐ *Side Note:*
NSUB1 through NSUB4 may range from 1 to 10, and each will divide the appropriate layer into equal sublayers. It should be noted that all application loads for a layer are applied to the uppermost sublayer.

☒ *Parameter Description:* **D4= thickness of the bottom soil layer (cm).**

☒ *Parameter Description:* **NSUB1= the number of sublayers in uppermost layer.**

☒ *Parameter Description:* **NSUB2= the number of sublayers in the second layer.**

☒ *Parameter Description:* **NSUB3= the number of sublayers in the third layer.**

☒ *Parameter Description:* **NSUB4= the number of sublayers in the bottom layer.**

☐ *Side Note:*
All sublayers have the same soil properties as the major soil layer in which they reside. However, the computed chemical concentrations in each sublayer will be different.

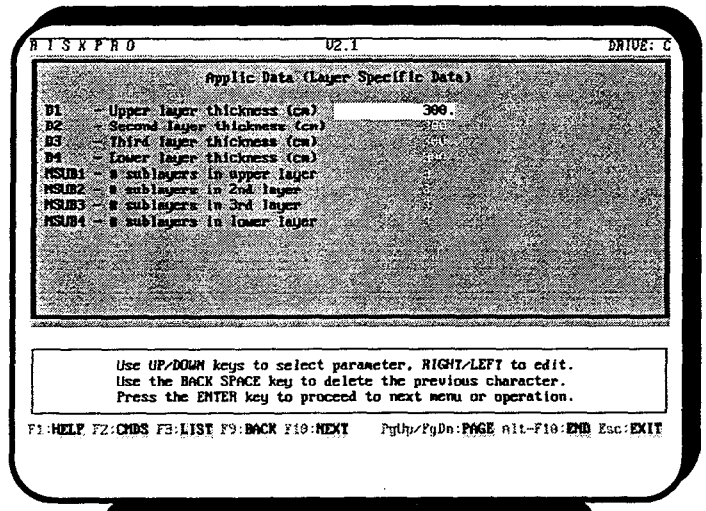
RISKPRO V2.1 DRIVE: C
Applic Data (Layer Specific Data)
D1 - Upper layer thickness (cm) 300.
D2 - Second layer thickness (cm)
D3 - Third layer thickness (cm)
D4 - Lower layer thickness (cm)
NSUB1 - # sublayers in upper layer
NSUB2 - # sublayers in 2nd layer
NSUB3 - # sublayers in 3rd layer
NSUB4 - # sublayers in lower layer
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 36
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 10** **Press the ENTER key to either accept the default data or the values you have input and to proceed to the next menu labeled *More APPLIC Data (Layer Specific Data)* (see Fig. 37).**

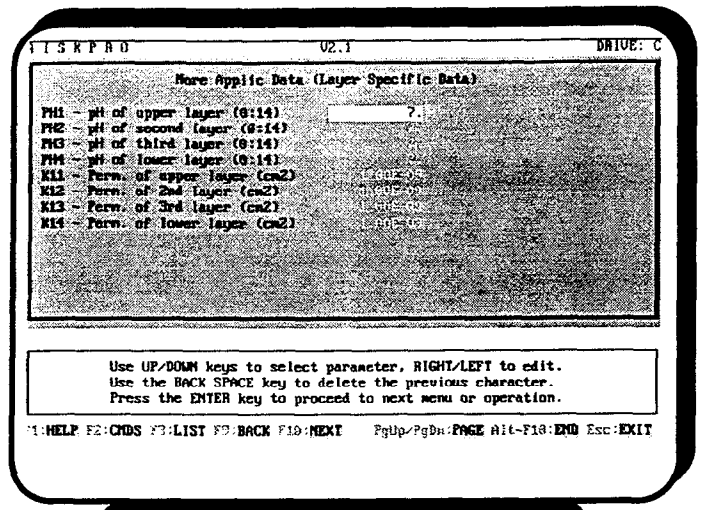
RISKPRO V2.1 DRIVE: C
More Applic Data (Layer Specific Data)
PH1 - pH of upper layer (0:14)
PH2 - pH of second layer (0:14)
PH3 - pH of third layer (0:14)
PH4 - pH of lower layer (0:14)
K11 - Perm. of upper layer (cm2)
K12 - Perm. of 2nd layer (cm2)
K13 - Perm. of 3rd layer (cm2)
K14 - Perm. of lower layer (cm2)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 37
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ *Side Note:*
pH is used only if the hydrolysis algorithm is used. Thus, if KNH, KAH, and KBH are 0.0 in the CHEM file, then you can ignore the pH values for the layers.

☑ **Step 11 As shown in Fig. 37, enter the PH1 through PH4 and K11 through K14 by highlighting each field with the up/down arrow keys. Note that:**

☒ *Parameter Description:* **PH1= the pH of the uppermost soil layer.**

☒ *Parameter Description:* **PH2= the pH of the second soil layer.**

☒ *Parameter Description:* **PH3= the pH of the third soil layer.**

☒ *Parameter Description:* **PH4= the pH of the bottom soil layer.**

☒ *Parameter Description:* **K11= the intrinsic permeability for the uppermost layer (cm^2).**

☐ *Side Note:*
If K1 (in the SOIL file) is set to zero, then K11, K12, K13, and K14 are used as the permeability values. If K1 from the SOIL data file is non-zero then K11, K12, K13 and K14 are not used, and should be set to zero. Refer to Sections 3.3, 3.5.2, and 3.5.9 where cautions are discussed for how the permeabilities are used in SESOIL.

☒ *Parameter Description:* **K12= the intrinsic permeability for the second layer (cm^2).**

☒ *Parameter Description:* **K13= the intrinsic permeability for the third layer (cm^2).**

☒ *Parameter Description:* **K14= the intrinsic permeability for the bottom layer (cm^2).**

☑ **Step 12 Next press the ENTER key to accept your input values and to proceed to the next menu labeled *Applic Data (Layer Ratios)* (see Fig. 38).**

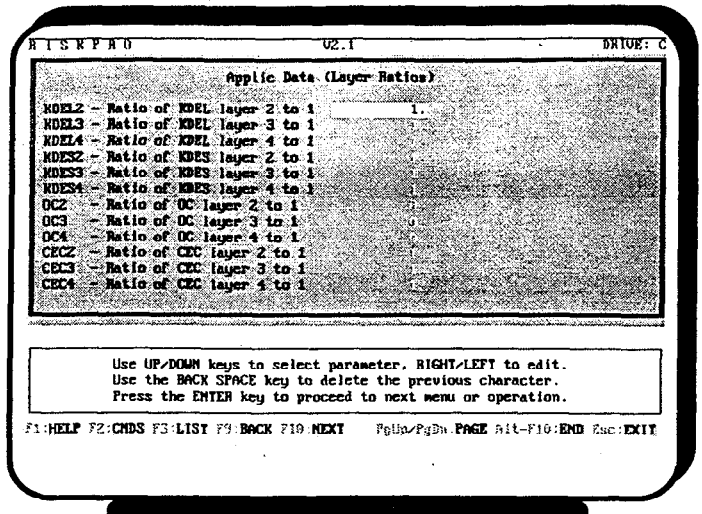
RISKPRO V2.1 DRIVE: C
Applic Data (Layer Ratios)
KDEL2 - Ratio of KDEL layer 2 to 1 1.
KDEL3 - Ratio of KDEL layer 3 to 1
KDEL4 - Ratio of KDEL layer 4 to 1
KDES2 - Ratio of KDES layer 2 to 1
KDES3 - Ratio of KDES layer 3 to 1
KDES4 - Ratio of KDES layer 4 to 1
OC2 - Ratio of OC layer 2 to 1
OC3 - Ratio of OC layer 3 to 1
OC4 - Ratio of OC layer 4 to 1
CEC2 - Ratio of CEC layer 2 to 1
CEC3 - Ratio of CEC layer 3 to 1
CEC4 - Ratio of CEC layer 4 to 1
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 38
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ ***Side Note:***
For example, the liquid phase biodegradation in layer 2 is computed as KDEL2 KDEL where KDEL is input in the CHEM file.*

☑ **Step 13 As shown in Fig. 38, you will be prompted to enter the following values where:**

☒ ***Parameter Description:*** **KDEL2= the ratio of KDEL (liquid phase biodegradation) in layer 2 to layer 1.**

☒ ***Parameter Description:*** **KDEL3= the ratio of KDEL (liquid phase biodegradation) in layer 3 to layer 1.**

☐ ***Side Note:***
KDEL and KDES are input in the CHEM file and OC and CEC are input in the SOIL file.

☒ ***Parameter Description:*** **KDEL4= the ratio of KDEL (liquid phase biodegradation) in layer 4 to layer 1.**

☒ ***Parameter Description:*** **KDES2= the ratio of KDES (solid phase biodegradation) in layer 2 to layer 1.**

☒ ***Parameter Description:*** **KDES3= the ratio of KDES (solid phase biodegradation) in layer 3 to layer. 1**

☒ ***Parameter Description:*** **KDES4= the ratio of KDES (solid phase biodegradation) in layer 4 to layer 1.**

☐ ***Side Note:***
The OC ratios are not used unless K in the CHEM file is 0.0, causing SESOIL to compute K using KOC and OC.

☒ ***Parameter Description:*** **OC2= the ratio of OC (organic carbon content) in layer 2 to layer 1. The organic carbon content usually decreases with depth.**

☒ ***Parameter Description:*** **OC3= the ratio of OC (organic carbon content) in layer 3 to layer 1. The organic carbon content usually decreases with depth.**

☒ *Parameter Description:* **OC4= the ratio of OC (organic carbon content) in layer 4 to layer 1. The organic carbon content usually decreases with depth.**

☒ *Parameter Description:* **CEC2= the ratio of CEC (cation exchange capacity) in layer 2 to layer 1.**

☒ *Parameter Description:* **CEC3= the ratio of CEC (cation exchange capacity) in layer 3 to layer 1.**

☒ *Parameter Description:* **CEC4= the ratio of CEC (cation exchange capacity) in layer 4 to layer 1.**

☑ **Step 14 After entering your values or accepting the default values given by the RISKPRO system, press the ENTER key to accept the ratio values and proceed to the next screen.**

☐ *Note: For most model runs, the user will use 1.0 for the ratios.*

☑ **Step 15 As shown in Fig. 39, this menu will prompt you to enter the final ratio values where:**

☐ *Side Note:*
FRN is input in the SOIL file. ADS is K from the CHEM file or KOC from the CHEM file if K is 0.0.

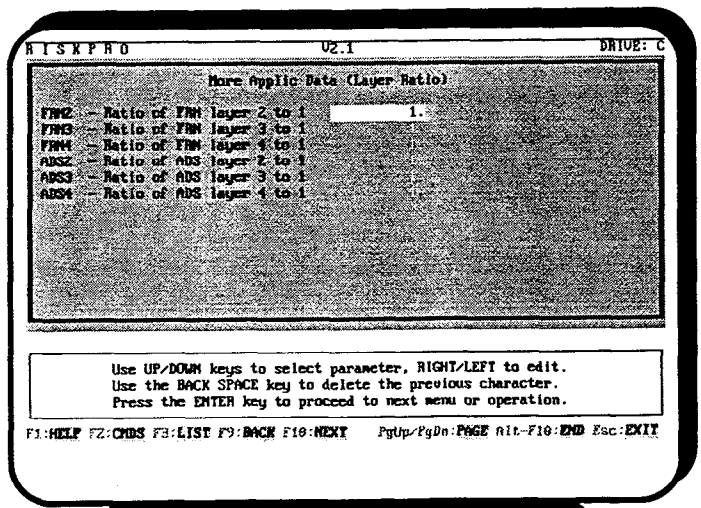
RISKPRO V2.1 DRIVE: C
More Applic Data (Layer Ratio)
FRN2 - Ratio of FRN layer 2 to 1 1.
FRN3 - Ratio of FRN layer 3 to 1
FRN4 - Ratio of FRN layer 4 to 1
ADS2 - Ratio of ADS layer 2 to 1
ADS3 - Ratio of ADS layer 3 to 1
ADS4 - Ratio of ADS layer 4 to 1
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 39
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ *Side Note:*
*Again, for example, the Freundlich exponent in layer 2 is computed as FRN2 * FRN where FRN is input in the SOIL file.*

☒ *Parameter Description:* **FRN2= the ratio of FRN (Freundlich exponent) in layer 2 to layer 1.**

☒ *Parameter Description:* **FRN3= the ratio of FRN (Freundlich exponent) in layer 3 to layer 1.**

☒ *Parameter Description:* **FRN4= the ratio of FRN (Freundlich exponent) in layer 4 to layer 1.**

☒ *Parameter Description:* **ADS2= the ratio of ADS (adsorption coefficient) in layer 2 to layer 1.**

☒ *Parameter Description:* **ADS3= the ratio of ADS (adsorption coefficient) in layer 3 to layer 1.**

☒ *Parameter Description:* **ADS4= the ratio of ADS (adsorption coefficient) in layer 4 to layer 1.**

☐ ***Technical Note:*** *If KOC (from the CHEM file) is used, these ratios (ADS2, ADS3, ADS4) should be set to 1.0 since KOC doesn't change. The calculated K_d is varied by the organic carbon content (see OC2, OC3, OC4 above). If K_d (K from the CHEM file) is used, the values can be varied with the ratios ADS2, ADS3, and/or ADS4.*

☑ **Step 16 After entering your values or accepting the default values given by the RISKPRO system, press the ENTER key to proceed to the next screen, the Applic Data (Pollutant Loading) for Layer 1, Year 1 menu (see Fig. 40).**

☐ ***Side Note:***
To move around in the pollutant loading menu the user should use the arrow keys to select the array element to edit, and Tab/Shift- and Tab key to move to the right and left data fields.

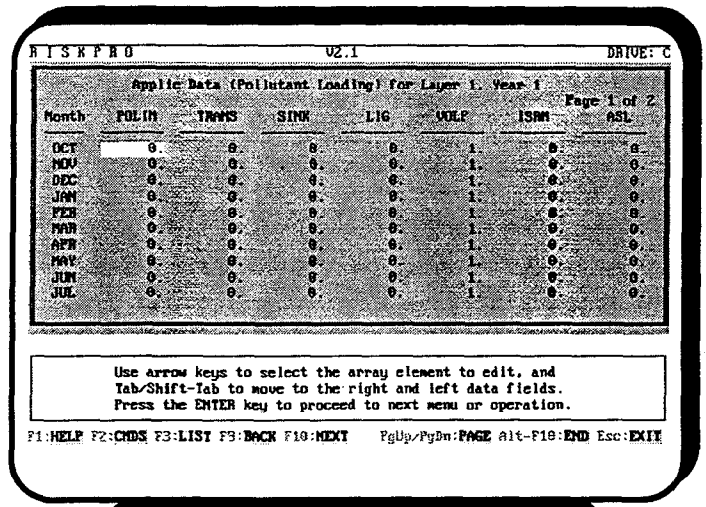
RISKPRO V2.1 DRIVE: C
Applic Data (Pollutant Loading) for Layer 1, Year 1 Page 1 of 2
Month POLIN TRANS SINK LIG VOLF ISRM ASL
OCT 0. 0. 0. 0. 1. 0. 0.
NOV 0. 0. 0. 0. 1. 0. 0.
DEC 0. 0. 0. 0. 1. 0. 0.
JAN 0. 0. 0. 0. 1. 0. 0.
FEB 0. 0. 0. 0. 1. 0. 0.
MAR 0. 0. 0. 0. 1. 0. 0.
APR 0. 0. 0. 0. 1. 0. 0.
MAY 0. 0. 0. 0. 1. 0. 0.
JUN 0. 0. 0. 0. 1. 0. 0.
JUL 0. 0. 0. 0. 1. 0. 0.
Use arrow keys to select the array element to edit, and
Tab/Shift-Tab to move to the right and left data fields.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 40
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1® copyright 1991.

☑ **Step 17 As shown in Fig. 40, this menu allows the user to enter an array of data for given parameters for each month where:**

☐ ***Side Note:***
See Section 3.5.2 for an explanation of how the pollutant depth is computed after POLIN is loaded into a sublayer.

☒ *Parameter Description:* **POLIN= the monthly pollutant load (mass per unit area) entering the top sublayer of the present soil zone (µg/cm²/month). If an initial soil-sorbed concentration is desired, a pollutant load may be applied at the beginning of the desired month to create the initial condition. The value of POLIN to specify may be calculated from the following equation: POLIN = CONC * L * RS where**

POLIN is the pollutant load to apply in µg/cm²/month, CONC is the concentration sorbed to the soil in µg/g or ppm, L is the thickness of the sublayer in centimeters which the pollutant is applied, and RS is the bulk density of the soil in g/cm³.

❑ ***Technical Note:*** *If ISPILL is 0, then the monthly load is applied continuously in 30 equal parts for the 30 time steps of the month. If ISPILL is 1, the total load is applied in the first time step of the month. See Section 3.5.2 for more details.*

☒ *Parameter Description:* **TRANS= the monthly mass of pollutant transformed in the present soil zone by processes not otherwise included in the model (µg/cm²/month).**

☒ *Parameter Description:* **SINK= the monthly mass of pollutant removed from the present soil zone by processes not otherwise included in the model (µg/cm²/month). For example, SINK could include an estimation of the amount of chemical in lateral flow.**

☒ *Parameter Description:* **LIG= the monthly input ligand mass to the present soil zone (µg/cm²/month).**

☒ *Parameter Description:* **VOLF= the index of volatilization/diffusion occurrence from the present soil zone. It may range from 0.0 to 1.0. VOLF = 0 means no volatilization/diffusion from this soil zone; VOLF = 1.0 means full volatilization/ diffusion allowed from this soil zone; VOLF = 0.5 means partial volatilization/diffusion (i.e. 50%) allowed from this soil zone (see Section 3.5.3).**

☒ *Parameter Description:* **ISRM= the index for pollutant transport in surface runoff. It may range from 0.0 to 1.0. ISRM is the ratio of the pollutant concentration in the surface runoff to the dissolved concentration in the top sublayer of the top soil layer. ISRM = 0.0 means no pollutant transport in surface runoff; ISRM = 0.40 means pollutant concentration in surface runoff is 0.40 times the concentration in the soil moisture of the top soil sublayer; ISRM = 1.0 means pollutant concentration in surface runoff equals the pollutant concentration in the soil moisture in the top sublayer (see Section 3.5.7).**

☒ *Parameter Description:* **ASL= the ratio of the pollutant concentration in rain to the pollutant's maximum solubility in water. That is , ASL is multiplied by SL (from the CHEM file) and the infiltration rate computed by the hydrologic cycle, and this result is entered in the top sublayer of layer 1.**

☐ *Note: Remember to use the page down key to enter the months of August and September.*

☑ **Step 18** **Once you have entered your array values listed above for Layer 1, Year 1 for each array parameter, press the ENTER key to proceed to the next menu option as shown in Fig. 41. Here you will see the same screen as in Fig. 40 except that now you are entering the values for Layer 2, Year 1.**

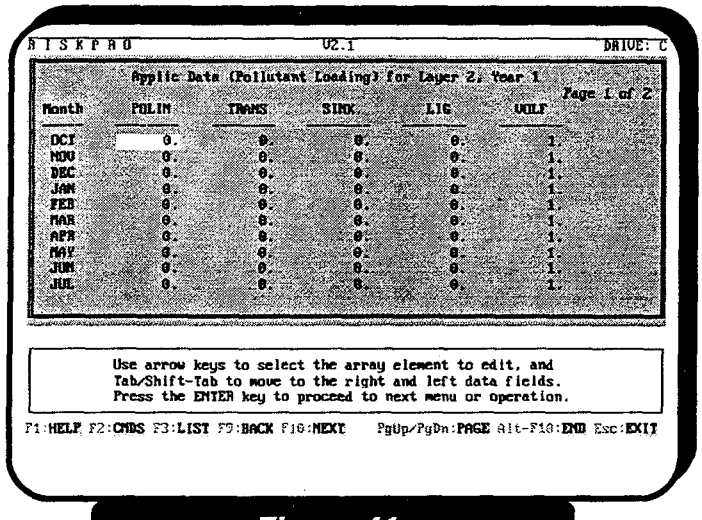
RISKPRO V2.1 DRIVE: C
Applic Data (Pollutant Loading) for Layer 2, Year 1 Page 1 of 2
Month POLIN TRANS SINK LIG VOLF
OCT 0. 0. 0. 0. 1.
NOV 0. 0. 0. 0. 1.
DEC 0. 0. 0. 0. 1.
JAN 0. 0. 0. 0. 1.
FEB 0. 0. 0. 0. 1.
MAR 0. 0. 0. 0. 1.
APR 0. 0. 0. 0. 1.
MAY 0. 0. 0. 0. 1.
JUN 0. 0. 0. 0. 1.
JUL 0. 0. 0. 0. 1.
Use arrow keys to select the array element to edit, and
Tab/Shift-Tab to move to the right and left data fields.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 41
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 19** **Press the ENTER key to accept the defaults of zero for each parameter (or 1.0 for VOLF) or repeat steps 17-18 to advance through each menu for each layer and year until all layers and years have the values you wish to input.**

☑ **Step 20** **After the final selection of pollutant input, RISKPRO will advance you to the next screen as shown in Fig. 42. This menu states that <u>You now have 1 year(s) of Monthly Application Data</u>. At this menu you have four options to choose from where:**

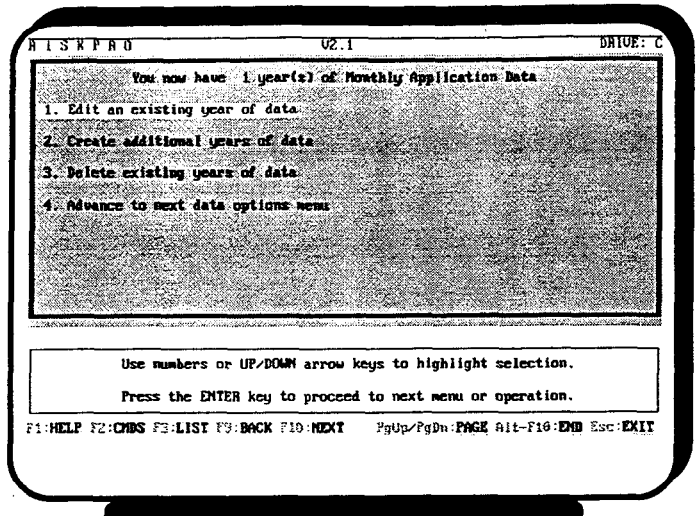
RISKPRO V2.1 DRIVE: C
You now have 1 year(s) of Monthly Application Data
1. Edit an existing year of data
2. Create additional years of data
3. Delete existing years of data
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 42
Screen courtesy of General Sciences Corporation's RISKPRO©, Version 2.1© copyright 1991.

☐ *OPTION 1* allows you to review and modify any year of existing data. If you choose option 1, you will be asked what year of pollutant data you wish to edit. If you have only one year of pollutant data you will be automatically placed into your only year of data to edit. Editing of this file is the same as before when you created the data.

☐ *OPTION 2* allows you to create more years of data, using any of the existing years. Note the total number of years of data you create does not necessarily have to equal the number of years you wish to simulate in your SESOIL run.

If the number of years of available data is less than the number of years specified for the SESOIL run (specified later; see Section 4.7), the model will automatically use the last year of available data for all remaining years of simulation during the model run.

If you choose this option you will be prompted to enter the number of additional years to create and the year of data to be used to create these data.

You must select a year of existing data which will be used to generate the additional years desired. You may then edit any or all of the newly created years of data.

☐ *OPTION 3* allows you to delete existing years of data. With this option you may delete existing years of data

by entering the number of years to be deleted. The last N years of existing data will be deleted (i.e., entering "5" deletes the last 5 years of existing data.) You may not delete all years of data; i.e., data for year 1 must always exist.

☐ *OPTION 4* advances you to the next menu selection.

☑ **Step 21** Once you have input your pollutant load(s) into the proper layer(s) and year(s) you may then selection option 4 to create the APPLIC file and advance to the next option menu (WASHLOAD menu).

4.5.2 Accessing A Default Data File For A Generic Municipal Landfill

As shown in Fig. 43, this option accesses default data for a generic municipal landfill. You may edit the default values to create your desired APPLIC data.

☑ **Step 1** **As shown in Fig. 43, highlight the option labeled Access generic municipal landfill data and press the ENTER key.**

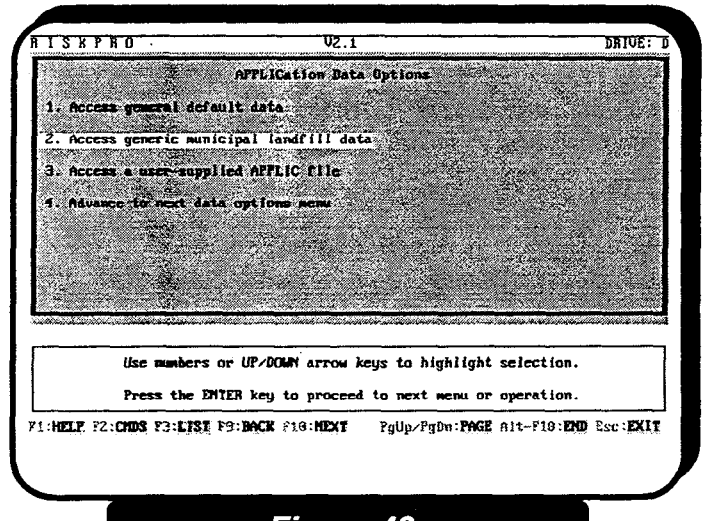
RISKPRO V2.1 DRIVE: D
APPLICation Data Options
1. Access general default data
2. Access generic municipal landfill data
3. Access a user-supplied APPLIC file
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 43
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **Repeat steps 2-21 in Section 4.5.1 to create and/or edit your APPLIC data file.**

4.5.3 Accessing A Previously Created APPLIC File

This option accesses a previously created APPLIC file. You may use the data as they are, or you may edit the data.

☑ **Step 1** **Highlight option 3 labeled Access a user-supplied APPLIC file and press the ENTER key as shown in Fig. 44.**

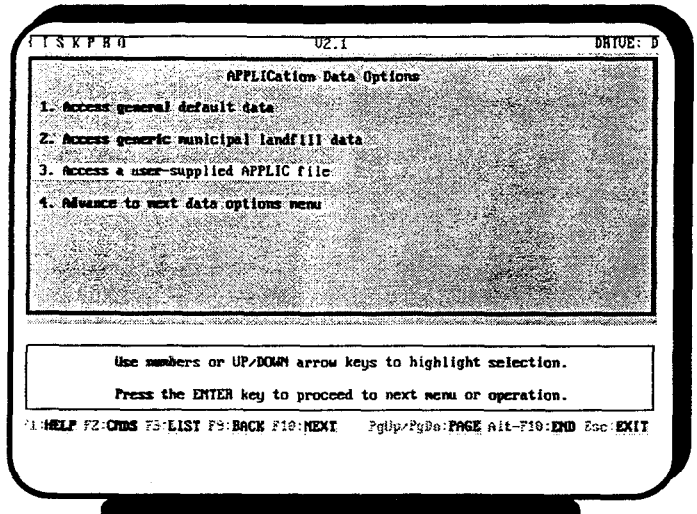
RISKPRO V2.1 DRIVE: D
APPLICation Data Options
1. Access general default data
2. Access generic municipal landfill data
3. Access a user-supplied APPLIC file
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 44
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 45, enter the file name for your APPLICATION data file. If no extension is specified, the extension ".INP" will be assumed. If using a file previously created by RISKPRO, the file name is of the form SAPPLxxx.INP, where xxx are three digits. You may press the F3 function key for a list of files in your catalog.**

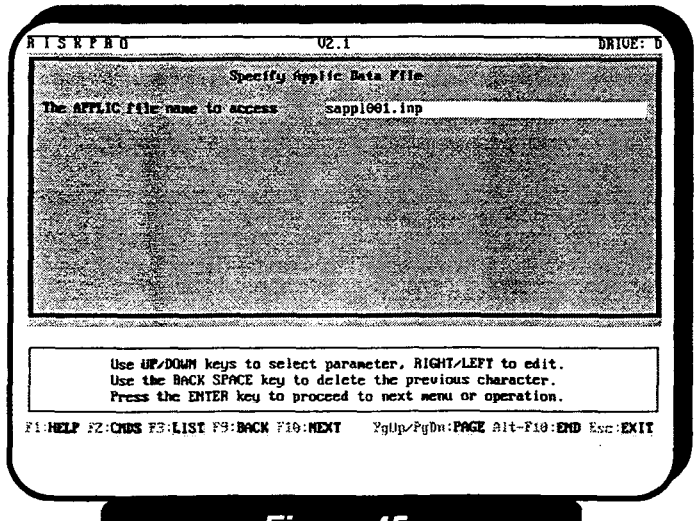
RISKPRO V2.1 DRIVE: D
Specify Applic Data File
The APPLIC file name to access sappl001.inp
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 45
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **Repeat steps 2-21 in Section 4.5.1 to create and/or edit your APPLIC file.**

4.5.4 Additional Information Regarding The APPLICATION File

❑ ***Technical Note:*** *In SESOIL, the user may specify a soil compartment with 2, 3, or 4 soil layers. The RISKPRO system prompts the user for data only for the number of layers that are specified.*

❑ ***Technical Note:*** *The application area may be the area of a landfill, a chemical spill, or a field receiving a chemical application.*

❑ ***Technical Note:*** *The latitude of the site is used in the calculation of potential solar radiation. It should correspond with the latitude of the site used to provide the climate data. If climate data are retrieved from the RISKPRO Climate Data Base, its latitude will automatically be entered in the APPLIC file. If, however, you access a user-supplied APPLIC file, be careful to input the correct latitude.*

❑ ***Technical Note:*** *In addition to specifying the thickness of each of the layers, the user may specify up to ten sublayers of each layer used. Sublayers will each be of equal thickness, and will have the same properties as the layer in which they reside.*

❑ ***Technical Note:*** *SESOIL requests data on pollutant release expressed as a monthly load. This loading may enter into any of the soil layers, or may enter the topsoil via rainfall. When a layer is broken into sublayers, the model assumes that the chemical loading enters the top sublayer and is immediately spread throughout this sublayer. Also see Section 3.5.2 for an explanation of how the pollutant depth is computed after a loading is entered.*

❑ ***Technical Note:*** *The model allows the user to specify either continuous or instantaneous release, as discussed above. Instantaneous releases assume that the total mass is loaded during the first time step of the month, and can be used to simulate spill loading (see Spill Index). However, this option applies only to the first layer. A continuous loading (the input loading divided by the number of time steps, 30, for each month) is always used for layers 2, 3, and/or 4 even if ISPILL is set to 1. See Section 3.5.2 for more details.*

❑ ***Technical Note:*** *When simulating a pollutant which undergoes complexation, the user must also provide a loading rate for the ligand which becomes part of the complex (parameter LIG). The parameters for pollutant transformed and pollutant removed (TRANS and SINK) are means for the user to include transformation and transport rates not specifically included in the SESOIL program. These parameters may be specified for each of the soil layers specified by the user.*

4.6 Creating the WASH File

The fifth input file to be created for a SESOIL run is the WASH file. The WASH file contains data used by SESOIL to calculate washload transport, the migration of the pollutant adsorbed to eroding soil particles. **Simulation of this process is optional.** If you do not wish to simulate washload, you do not need to create the WASH file. As shown in Fig. 46, RISKPRO will prompt you to enter a YES to specify washload data, or NO to omit it. If you enter a YES, you will be prompted

to continue to build the WASH file. If you enter a NO, all inputs for the SESOIL run will have been completed.

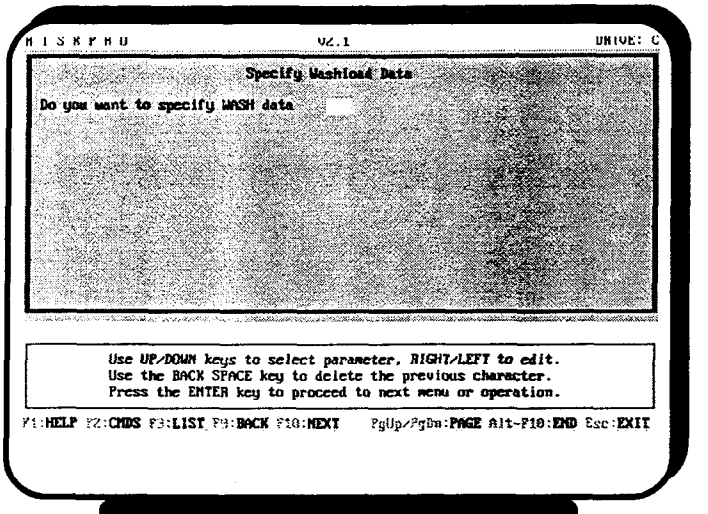
R I S K P R O
V2.1
DRIVE: C
Specify Washload Data
Do you want to specify WASH data
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 46
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

❑ ***Technical Note:*** *Note that surface runoff, in which dissolved pollutant may be transported as part of overland flow of rainwater, is simulated by SESOIL as part of the pollutant cycle only if ISRM (in the APPLIC file) does not equal 0. Chemicals having high adsorption coefficients are likely to be carried with eroding soil. A good introductory application may be found in Hetrick & Travis (1988).*

There are several options available for obtaining or entering the required data (see Fig. 47). The following describes each menu option:

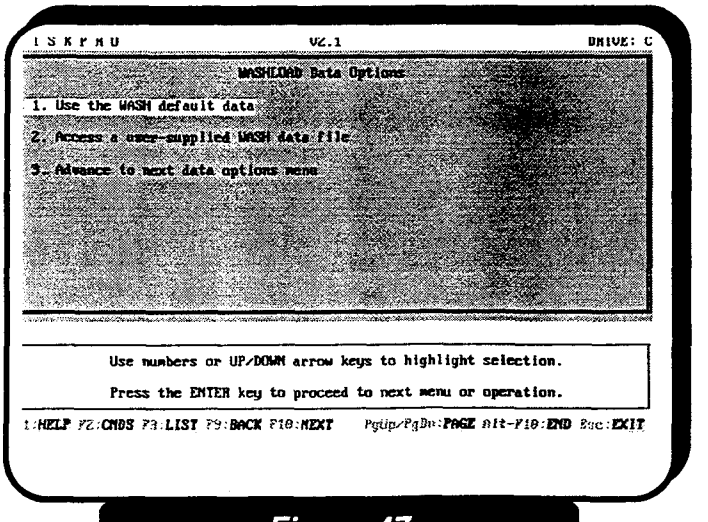
R I S K P R O
V2.1
DRIVE: C
WASHLOAD Data Options
1. Use the WASH default data
2. Access a user-supplied WASH data file
3. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 47
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

❑ *OPTION 1* **accesses the WASHLOAD default data. You may edit data as desired to create your desired dataset. This option is discussed in Section 4.6.1.**

☐ *OPTION 2* **accesses a user-specified WASHLOAD data file. You may use this option only if you have previously created the WASH data as is discussed in Section 4.6.5.**

☐ *OPTION 3* **exits from the WASH data option.**

For options 1 or 2, the user may tailor the data for the chosen scenario. Several years of data may be entered at this point, or the user may provide one year of data. Table 4.8 below lists the data required for this file.

Table 4.8
WASHLOAD PARAMETERS

Symbol	Parameter Description
ARW	Washload Area (cm^2)
SLT	Silt Fraction
SND	Sand Fraction
CLY	Clay Fraction
SLEN	Slope Length (cm)
SLP	Average Land Slope (cm/cm)
KSOIL	Soil Erodibility Factor (tons/acre/English EI)
CFACT	Soil Loss Ratio (unitless)
PFACT	Contouring Factor (unitless)
NFACT	Manning's Coefficient (unitless)

4.6.1 Using And Creating The WASH Default Data File Option

☑ **Step 1** **Choose the option labeled Use the WASH default data and press the ENTER key.**

☑ **Step 2** **As shown in Fig. 48 enter a descriptive label for the WASH data file (up to 20 characters). This label will appear in the file catalog manager and is used to identify the input file.**

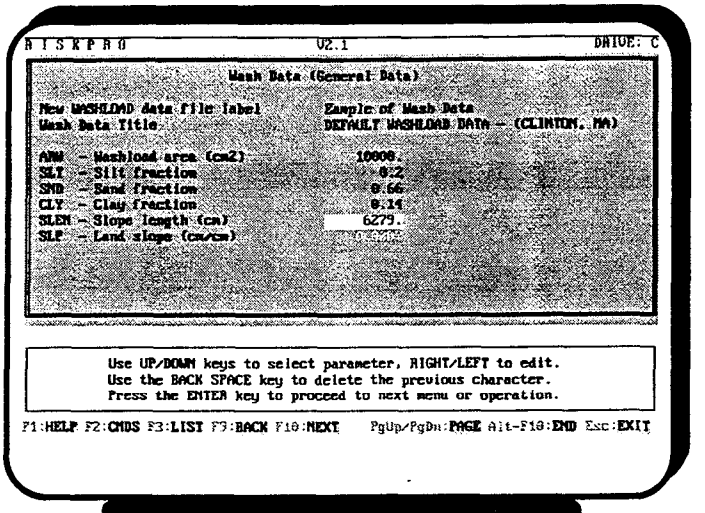
RISKPRO V2.1 DRIVE: C
Wash Data (General Data)
New WASHLOAD data file label
Wash Data Title
Example of Wash Data
DEFAULT WASHLOAD DATA - (CLINTON, MA)
AWW - Washload area (cm2) 10000.
SLT - Silt fraction 0.2
SND - Sand fraction 0.66
CLY - Clay fraction 0.14
SLEN - Slope length (cm) 6279.
SLP - Land slope (cm/cm)
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 48
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **Use your down arrow key to highlight the descriptive title field for your WASHLOAD data. Enter up to 48 characters to describe the WASHLOAD data file. This title field will appear in the output report file.**

☑ **Step 4** **Next highlight each field where you will be prompted to enter the following values :**

☐ *Side Note:*
The washload area required in the WASH file refers to a patch of topsoil subject to erosion. The area of this patch can be smaller than or equal to the application area for the simulation run. The silt, sand, and clay fractions refer to this layer of topsoil; this soil need not have the same properties as the upper layer of soil in the soil column. SESOIL also requires information about the land over which the surface runoff and the washload will travel, including the length of the slope between the washload area and a barrier or sink into which the runoff will drain, and the

☒ *Parameter Description:* **ARW= the washload area (cm^2). ARW should be equal to or less than the Application area AR when pollutant transport in the washload is of concern.**

☒ *Parameter Description:* **SLT= the fraction of silt in the soil. Note: The sum of SLT, SND and CLY must add up to 1.0.**

☒ *Parameter Description:* **SND= the fraction of sand in the soil. Note: The sum of SLT, SND and CLY must add up to 1.0.**

☒ *Parameter Description:* **CLY= the fraction of clay in the soil. Note: The sum of SLT, SND and CLY must add up to 1.0.**

☒ *Parameter Description:* **SLEN= the slope length (length of travel) of the representative overland flow profile (cm).**

☒ *Parameter Description:* **SLP= the average slope (cm/cm) of the representative overland flow profile.**

☐ ***Side Note:***
At Step 5, default values are given for all remaining parameters (KSOIL, CFACT, PFACT, NFACT) in the WASH file (see Section 4.6.2 below). These values should be changed for the site being studied.

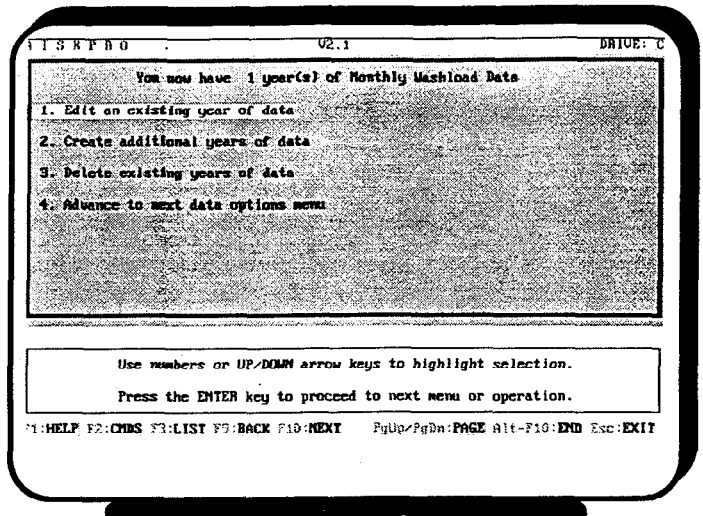
RISKPRO V2.1 DRIVE: C
You now have 1 year(s) of Monthly Washload Data
1. Edit an existing year of data
2. Create additional years of data
3. Delete existing years of data
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 49
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 5** **After entering values for each of the above parameters press the enter key to advance to the next menu as shown in Fig. 49. This menu states that <u>You now have 1 year(s) of Monthly Washload Data</u>. At this menu you have four options to choose from where:**

- ☐ ***OPTION 1*** **will allow you to review and modify any year of existing WASH data (see Section 4.6.2).**
- ☐ ***OPTION 2*** **allows you to create more years of data, using any of the existing years. The total number of years of data you create does not necessarily have to equal the number of years you wish to simulate in your SESOIL run. If the number of years of available data is less than the number of years specified for the SESOIL run, the model will automatically use the last year of available data for all remaining years of simulation (see Section 4.6.3).**
- ☐ ***OPTION 3*** **allows you to delete existing years of WASH data (see Section 4.6.4).**
- ☐ ***OPTION 4*** **allows you to finish creating your WASH data . By selecting this option you will create the WASHLOAD file and have completed building the SESOIL data files. You will be informed by RISKPRO that SWASH###.INP has been successfully inserted into your catalog file system.**

4.6.2 Editing An Existing Year Of Data

☑ Step 1 **Choose the first option, as shown in Fig. 49, to review and modify any year of existing data. By choosing this menu option, you will be prompted to modify arrays of washload data factors for year 1 as shown in Fig. 50. The parameters and their definitions are:**

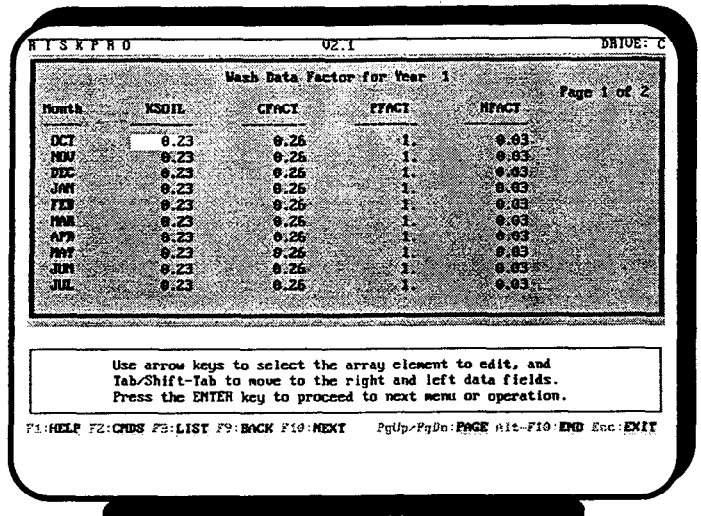
RISKPRO V2.1 DRIVE: C
Wash Data Factor for Year 1
Page 1 of 2
Month KSOIL CFACT PFACT NFACT
OCT 0.23 0.26 1. 0.03
NOV 0.23 0.26 1. 0.03
DEC 0.23 0.26 1. 0.03
JAN 0.23 0.26 1. 0.03
FEB 0.23 0.26 1. 0.03
MAR 0.23 0.26 1. 0.03
APR 0.23 0.26 1. 0.03
MAY 0.23 0.26 1. 0.03
JUN 0.23 0.26 1. 0.03
JUL 0.23 0.26 1. 0.03
Use arrow keys to select the array element to edit, and
Tab/Shift-Tab to move to the right and left data fields.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 50
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☒ *Parameter Description:* **KSOIL= the soil erodibility factor (tons/acre/English EI) used in the Universal Soil Loss Equation. Its value typically ranges from 0.03 to 0.69; the default value is 0.23.**

☐ *Side Note:* *Examples of the washload parameters can be found in the CREAMS documentation (Knisel, 1980; Foster et al., 1980)*

☒ *Parameter Description:* **CFACT= the soil loss ratio (unitless) used in the Universal Soil Loss Equation. It depends on the cover and management of the land. Its value typically ranges from 0.0001 (well managed) to 0.94 (tilled); the default value is 0.26.**

☒ *Parameter Description:* **PFACT= the contouring factor for agricultural land. This factor ranges from 0.1 (extensive practices) to 1.0 (no supporting practice); the default value is 1.0.**

☒ *Parameter Description:* **NFACT= Manning's coefficient (unitless) for overland flow as used in the Universal Soil Loss Equation. Its value typically ranges from 0.01 to 0.40; the default value is 0.03.**

☑ **Step 2** **The array values can be modified by using the arrow keys to edit the array element for each month, and/or the Tab/Shift-Tab to move to the right and left data fields. When you are done editing the data, press the ENTER key to accept your data. RISKPRO will display a menu stating You now have 1 year(s) of Monthly Washload Data as shown in Fig. 51.**

4.6.3 Creating Additional Years Of Data

☑ **Step 1** **As shown in Fig. 51, highlight option 2 labeled *Create additional years of data* and press the ENTER key.**

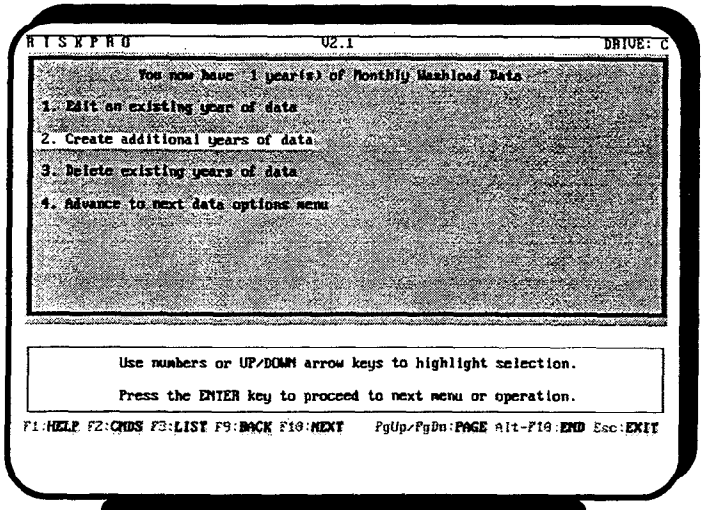
RISKPRO V2.1 DRIVE: C
You now have 1 year(s) of Monthly Washload Data
1. Edit an existing year of data
2. Create additional years of data
3. Delete existing years of data
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 51
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **The next menu will prompt you to enter the number of years to create and the year of data to use to create the data. (see Fig. 52). Enter a value for each field and press the ENTER key to advance to the next menu.**

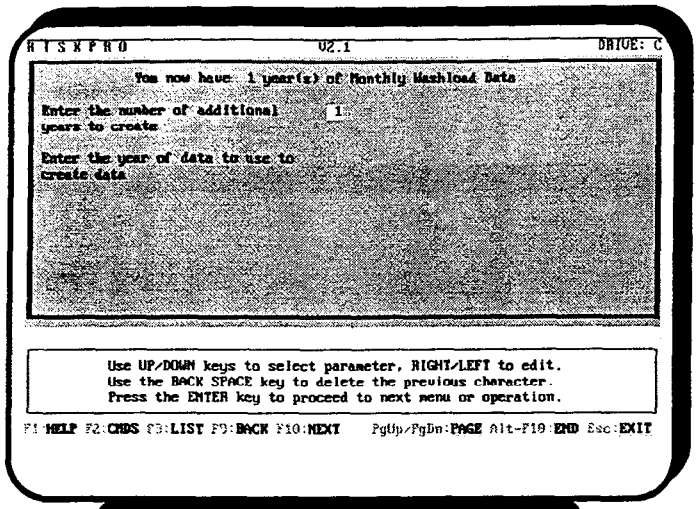
RISKPRO
V2.1
DRIVE: C
You now have 1 year(s) of Monthly Washload Data
Enter the number of additional years to create
1
Enter the year of data to use to create data
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 52
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1™ copyright 1991.

☑ **Step 3** **Your menu will tell you that you have created additional years of monthly washload data and will allow you to either edit the data, create more years of data, delete existing years of data, or advance to the next menu.**

❑ ***Technical Note:*** *If only one year of data exists, then year 1 must be used to generate the remaining years. If more than one year exists, you may choose any existing year of data to be used to create the additional years. The additional years created can then be further modified if so desired. The total number of years of data you create does not necessarily have to equal the number of years you wish to simulate in your SESOIL run. If the number of years of available data is less than the number of years specified for the SESOIL run, the model will automatically use the last year of available data for all remaining years of simulation during the model run.*

❑ ***Technical Note:*** *Remember for the second option here, you must select a year of existing data which will be used to generate the additional years desired. You may then edit any or all of the newly created years of data if desired. Repeat steps 1-2 in Section 4.6.2 to work with your WASHLOAD data file.*

4.6.4 Deleting An Existing Year Of WASH Data

☑ **Step 1** **As shown in Fig. 53, highlight the option labeled Delete existing years of data and press the ENTER key.**

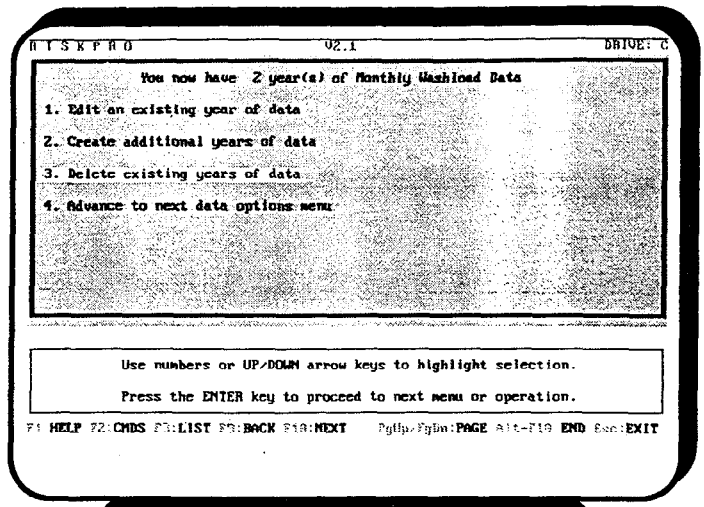
RISKPRO V2.1 DRIVE: C
You now have 2 year(s) of Monthly Washload Data
1. Edit an existing year of data
2. Create additional years of data
3. Delete existing years of data
4. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1 HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10 END Esc:EXIT

Figure 53
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ ***Side Note:***
The user should note that this option can not selectively delete a particular year of data as shown in Figure 54.

☑ **Step 2** **Enter the numbers of years of data you wish to delete (see Fig. 54) and press the ENTER key to return to the same menu selection (see Fig. 53). The last N years of existing data will be deleted.**

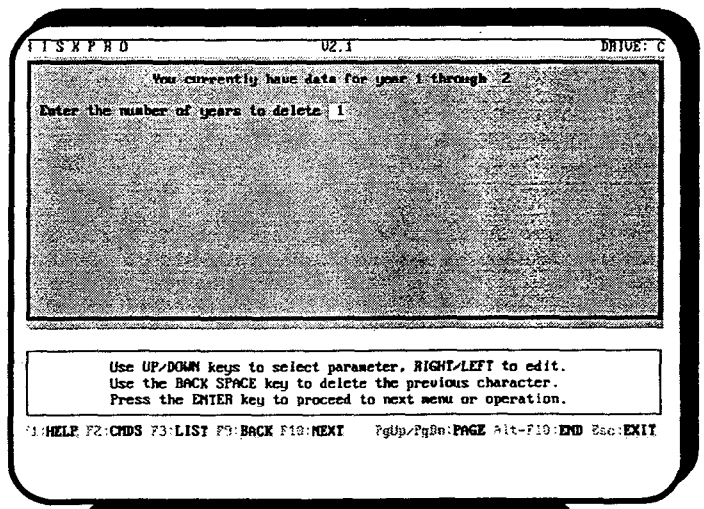
RISKPRO V2.1 DRIVE: C
You currently have data for year 1 through 2
Enter the number of years to delete 1
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 54
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

4.6.5. Accessing A User-Supplied WASH Data File

☑ **Step 1** **From the WASHLOAD Data Option menu highlight the option labeled Access a user-supplied WASH data file and press the ENTER key as shown in Fig. 55 .**

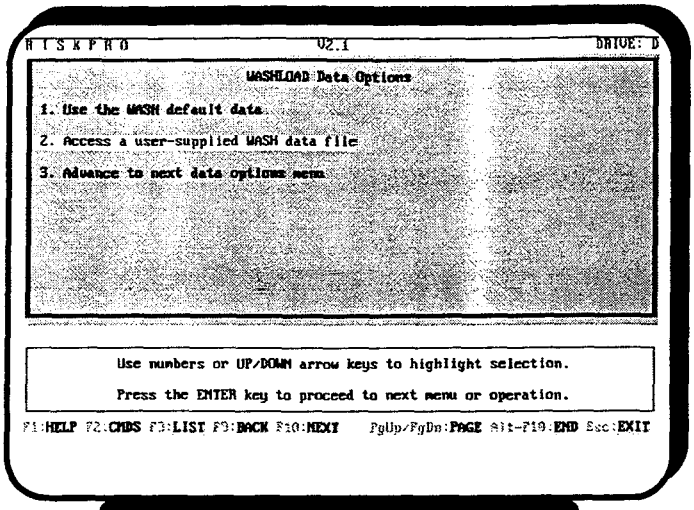
RISKPRO V2.1 DRIVE: D
WASHLOAD Data Options
1. Use the WASH default data
2. Access a user-supplied WASH data file
3. Advance to next data options menu
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 55
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **In Fig. 56 you will be prompted to enter the file name for your WASHLOAD data file. If no extension is specified, the extension ".INP" will be assumed. The file name is of the form SWASHxxx.INP, where xxx are three digits. You may press the F3 function key for a list of files in your catalog.**

☑ **Step 3** **Repeat any of the steps in Sections 4.6.2 through 4.6.4 to edit the data or create or delete any additional years of data.**

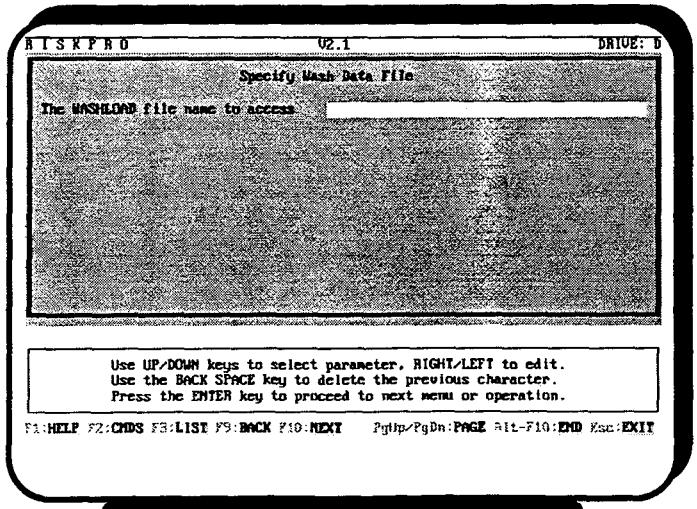
RISKPRO V2.1 DRIVE: D
Specify Wash Data File
The WASHLOAD file name to access
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 56
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

4.7 Running the SESOIL Model

To run the SESOIL model, you must specify the five SESOIL input files for your SESOIL run: CLIMATE, SOIL, CHEM, APPLIC and WASH. The WASH file is optional and need be specified only if washload simulation is to be performed. The EXEC file, which contains SESOIL run control parameters, is automatically created by the SERUN program, and therefore need not be specified. The default names are the last ones that were created by SEBUILD in RISKPRO. The run files created in RISKPRO are stored in the catalog manager and a list of files can be retrieved using the F3 key.

☑ **Step 1** **As shown in Fig. 57, select option 2, labeled SERUN, and press the ENTER key.**

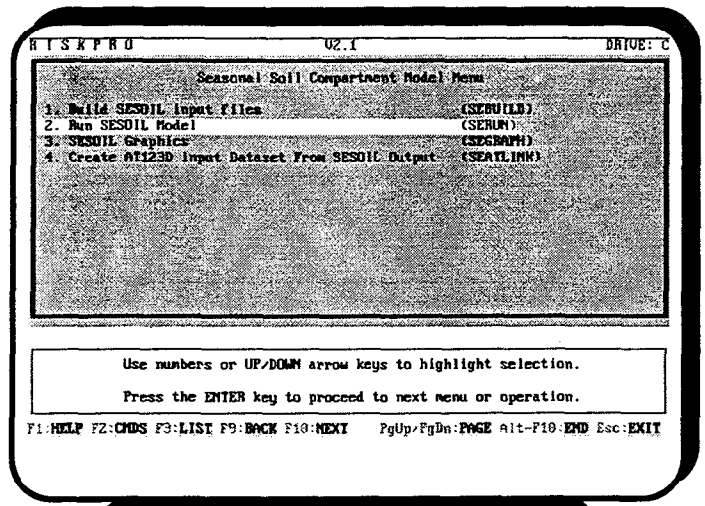
RISKPRO V2.1 DRIVE: C
Seasonal Soil Compartment Model Menu
1. Build SESOIL input files (SEBUILD)
2. Run SESOIL Model (SERUN)
3. SESOIL Graphics (SEGRAPH)
4. Create AT123D Input Dataset From SESOIL Output (SEATLINK)
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 57
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **Enter the file names for your CLIMATE, SOIL, CHEM, APPLIC, and WASH data files. If no extension is specified, the extension ".INP" will be assumed as shown in Fig. 58. Note that the WASH data file is optional. If washload is not to be simulated, enter "NONE". Remember to use your F3 key to list files from the contents of your active catalog file. Press the ENTER key to advance to the next menu option.**

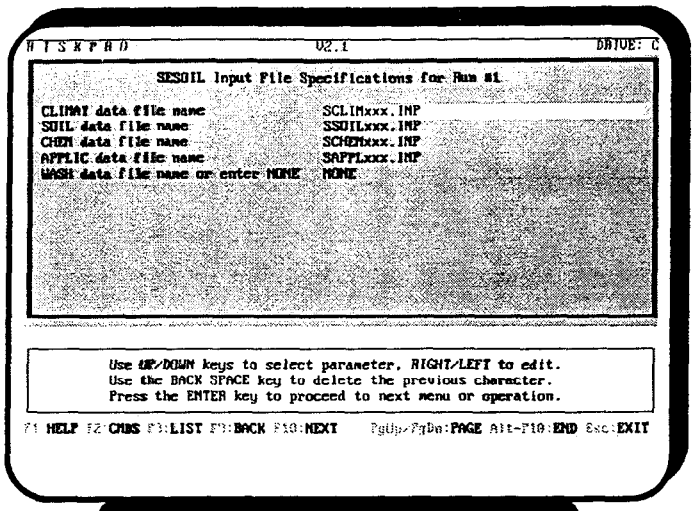
R I S K P R O
V2.1
DRIVE: C
SESOIL Input File Specifications for Run #1
CLIMAT data file name
SCLIMxxx.INP
SOIL data file name
SSOILxxx.INP
CHEM data file name
SCHEMxxx.INP
APPLIC data file name
SAPPLxxx.INP
WASH data file name or enter NONE
NONE
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1 HELP F2:CHBS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 58
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **As shown in Fig. 59, enter a label for the output report file, which appears in the catalog manager. It is used to identify your output files. The same label will be applied to the report file (.OUT), the results file (.RES), and the AT123D linkage file (.ATX). You may enter up to 20 characters.**

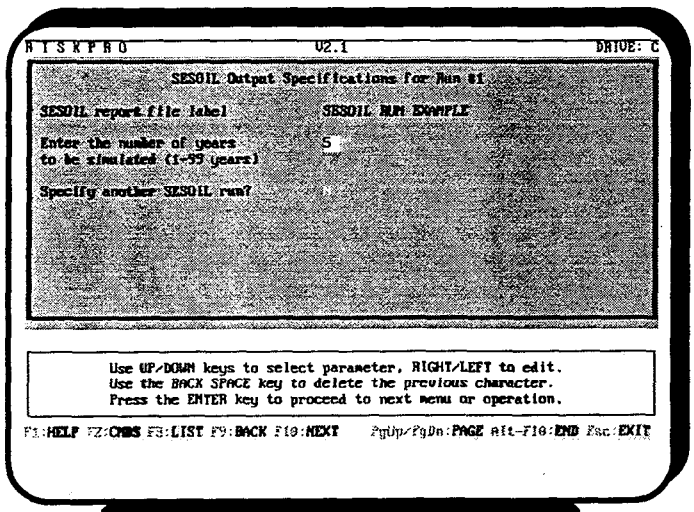
R I S K P R O
V2.1
DRIVE: C
SESOIL Output Specifications for Run #1
SESOIL report file label
SESOIL RUN EXAMPLE
Enter the number of years to be simulated (1-99 years)
5
Specify another SESOIL run?
N
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CHBS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 59
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 4** **Next hit the down arrow key to highlight the option labeled *Enter the number of years to be simulated (1-99 years)*. Enter the number of years to be simulated for this model run.**

❑ ***Technical Note:*** *Remember the number of years simulated does not have to be equal to the number of years of data available in the input files. When it is set higher than the number of years of available data for the CLIMATE, APPLIC and WASH data files, the last year of available data in each of these data files is*

repeated for the remaining years during the SESOIL run. When the number of years to be simulated is less than the number of years in the data files, the remaining years of data are ignored during the SESOIL run. Up to 99 years may be simulated.

☑ **Step 5** **Next select the specify run option. Enter "Y" if you wish to specify another SESOIL run, and to repeat steps 2 - 4 to create another model run. Otherwise enter "N" to begin model execution. All SESOIL model runs will be performed in sequence.**

☑ **Step 6** **If the model has run successfully you should see an output screen of a model run as shown in Fig. 60. After reviewing the output file press the ALT- F10 key. RISKPRO will insert three output files into your active catalog manager and label them as SSOUTxxx.OUT, SSOUTxxx.RES, and SSOUTxxx.ATX.**

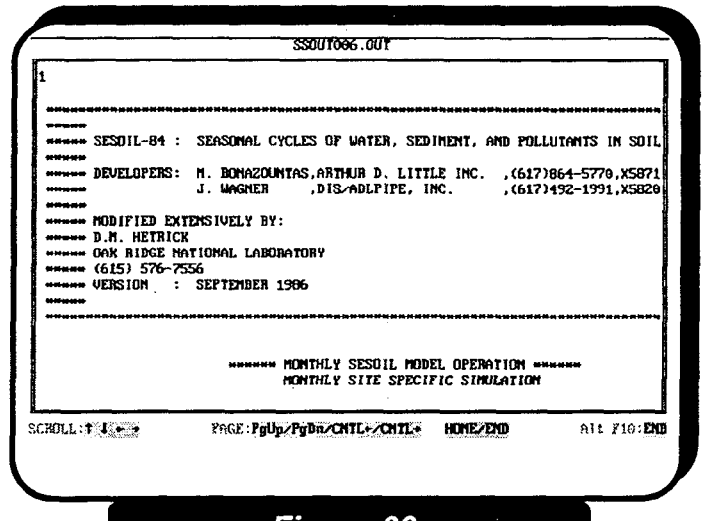
SSOUT086.OUT
1
SESOIL-84 : SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL
DEVELOPERS: M. BONAZOUNTAS,ARTHUR D. LITTLE INC. ,(617)864-5770,X5871
J. WAGNER ,DIS/ADLPIPE, INC. ,(617)492-1991,X5820
MODIFIED EXTENSIVELY BY:
D.M. METRICK
OAK RIDGE NATIONAL LABORATORY
(615) 576-7556
VERSION : SEPTEMBER 1986
****** MONTHLY SESOIL MODEL OPERATION ******
MONTHLY SITE SPECIFIC SIMULATION
SCROLL:↑↓←→ PAGE:PgUp/PgDn/CNTL+/CNTL+ HOME/END Alt F10:END

Figure 60
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

❑ ***Technical Note:*** *If only one run is specified, the output report will automatically be displayed at the completion of the run. If more than one run is specified, the runs are set up in batch mode and the output reports will not be displayed at the completion of the runs, but may be viewed by running the Catalog Manager under the "Data Management" menu.*

❑ ***Technical Note:*** *Refer to appendix B to see an example of a SESOIL output report file that resulted from using the example data given in Appendix A.*

❑ ***Technical Note:*** ***SSOUTxxx.OUT*** *is an ASCII file of the SESOIL output report (see Appendix B).*

❑ ***Technical Note:*** ***SSOUTxxx.RES*** *is an input file used by the graphics program SEGRAPH. The SESOIL model results from this file allows you to create the graphics from a SESOIL model run.*

❑ ***Technical Note:*** ***SSOUTxxx.ATX*** *is an input file for the AT123D model. The SESOIL model results are stored in this file and have the extension "ATX". Note that the ATX file will not be further discussed in this report.*

Reviewing and Using SESOIL Results

5

SESOIL model output are accessible in two ways from RISKPRO: (1) a report file that includes a summary of the input data used in the simulation and the monthly results from the model, and (2) an output data set that contains selected results from SESOIL that can be used by the RISKPRO graphing program. The SESOIL report file is explained in Section 5.1 and Section 5.2 describes the graphing capabilities. While reading Section 5.1, refer to Appendix B which contains a report file that resulted from using the example data shown in Appendix A.

5.1 The SESOIL Output Report File

The SESOIL report file contains the model input and monthly results from the hydrologic cycle, washload cycle (if used), and pollutant cycle. An annual summary report is also printed for each year. As can be seen in Appendix B, this file can be quite lengthy. For example, a ten-year simulation that includes all four layers with three sublayers per layer will produce an output report file that requires approximately 250000 bytes of storage on an IBM (or compatible) personal computer. Thus, multiple runs could require significant disk space.

5.1.1 Output Of The Model's Input

The first section of the file contains a summary of the site followed by a list of the input used by the model. The input is subdivided into soil, chemical, washload (if used), and application data. The next table (labeled "YEAR - 1 MONTHLY INPUT PARAMETERS") reports the monthly climatic data, the pollutant input parameters for each month, and the monthly washload factors (if used) for the first year. Since all the input data were described thoroughly earlier in this report (see Section 4), they will not be discussed further here.

Following the data for the first year, the monthly input parameters for the climate, pollutant, and washload are given for each year. If the data for any of these categories (i.e., climatic, pollutant, or washload) are the same as the previous year, they are not printed, but a message is given stating, for example, "-- CLIMATIC INPUT PARAMETERS ARE SAME AS LAST YEAR." This is common when long-term monthly averaged data are used. See Appendix B for examples.

The user should check this section of the output report file carefully to ensure that the input data are correct or to see if there are other warning messages. SESOIL checks to see if there are any obvious errors in the data and, if there are, error or warning messages will be printed to the user immediately before the section entitled "GENERAL INPUT PARAMETERS." For example, the fraction of cloud cover must always be between 0.0 and 1.0 and an error message is printed if it is

not. Also, immediately after the input data are printed and just before the monthly hydrologic results are output (i.e., before the section entitled "YEAR - 1 MONTHLY RESULTS (OUTPUT)"), any additional warnings or errors that SESOIL recognizes are printed. For example, warnings or errors that occur during the hydrologic cycle calculations will be printed here. For the user's convenience, all error and warning messages and their meanings are listed in Appendix C.

5.1.2 Output Of The Model's Monthly Results

The next section of the output file reports the model results, which are divided into annual subsections. These data are grouped by the year simulated, with the results reported for each month. The monthly results are organized in the following order:

- **Hydrologic cycle components**
- **Washload cycle components (if used)**
- **Pollutant mass input**
- **Pollutant mass distribution for each layer (sublayer)**
- **Pollutant concentration distribution for each layer (sublayer)**
- **Pollutant depth**

These monthly results are followed by an annual summary. The following discusses each category in detail.

The results for each year begin with the monthly results for the hydrologic cycle. The first parameter printed, labeled "MOIS. IN L1 (%)" (see Appendix B), is the volumetric soil moisture content in the root zone, defined in SESOIL as the first 100 cm of the unsaturated soil zone. The next parameter, labeled "MOIS. BELOW L1 (%)", is the average volumetric soil moisture content for the entire soil column (from the surface to the groundwater table). Notice that in the example output file (Appendix B) these two parameters are the same for each month. The hydrologic cycle of SESOIL needs further development before there will be any significant difference between these two parameters since an average permeability is used for the entire soil column in the hydrologic cycle. At present, only very dry climates may cause a difference (Bonazountas, personal communication, 1986).

The calculated precipitation in units of cm (labeled "PRECIPITATION (CM)") is listed next for each month. (As stated in Section 3.3, the program iterates on the soil moisture in equations (1) and (2) until the calculated precipitation compares well with the measured precipitation input by the user.) This result is followed by

the infiltration, the evapotranspiration, the moisture retention, the surface runoff, and the groundwater runoff (recharge), all in units of cm. Infiltration is calculated as the difference between the precipitation and the surface runoff, and is also equal to the moisture retention plus the evapotranspiration plus the groundwater runoff (recharge). The yield is simply the surface runoff plus the groundwater runoff (recharge). The next two lines, "PAU/MPA (GZU)" and "PA/MPA (GZ)", are the calculated precipitation for each month for the root zone and the entire soil column, respectively, each divided by the measured precipitation. Refer to Section 3.3 where more details are given on the hydrologic cycle components.

Following the hydrologic cycle results, the next table in the output file contains the monthly results from the washload cycle if this option was used (the model run that produced the example output file in Appendix B did not use this option). The sediment yield is given on the first two lines in kg/km^2 and g/cm^2, respectively (labeled as "WASHLD (KG/SQ KM)" and "(G/SQ CM)"). The next line, labeled "ENRICHMT RATIO (-)", is defined as the ratio of the total specific surface area for the sediment and organic matter to that of the original soil (Knisel et al., 1983). The index of specific surface is given as m^2/g of total sediment and is labeled "SURF. IDX (M**2/G)" (see Knisel et al., 1983). Next, the relative amounts of clay, silt, and sand in the eroded particles are given, labeled as "SED. FRAC CLAY," "SED. FRAC SILT," and "SED. FRAC SAND." These three numbers add to 1.0 for each month. The last line given for the washload results is labeled "SED. FRAC OC" and is the fraction of organic matter in the eroded sediment. Refer to Section 3.4 which describes the washload cycle in more detail.

The pollutant mass input, in units of µg, is the next table in the output file. These values include the amount of chemical (µg) in the precipitation (labeled "PRECIP.") and the amount loaded into each of up to four major layers specified in the simulation, labeled "LOAD UPPER," "LOAD ZONE 2," "LOAD ZONE 3," and "LOAD LOWER." PRECIP is computed by multiplying ASL (input parameter from the APPLIC file described in Section 4.5), by SL (input parameter from the CHEM file described in Section 4.4), by the infiltration rate computed by the hydrologic cycle, and by the area of application (input parameter AR from the APPLIC file). For the loads in each layer, the values are simply the area of application (input parameter AR) multiplied by the pollutant application (input parameter POLIN for each layer from the APPLIC file). Note that if there are sublayers within the major layers, then the load listed for the major layer is added to the first sublayer of that layer, not evenly for each of the sublayers. If a spill loading was specified (see the line labeled "SPILL (1) OR STEADY APPLICATION (0):" under "-- APPLICATION INPUT PARAMETERS --") the input listed for the month for the surface layer is loaded into the layer in the first time step of the month. If steady loading was specified, the input for the month is spread out evenly during each time step of the month. Note that a spill loading applies only to the first layer. (Refer to Sections 3.5.2 and 4.5 for more details.) The total input to the soil column is given next (labeled "TOTAL INPUT") and is simply the total sum of all inputs for a given month.

The next table printed in the output file gives the distribution of pollutant mass in µg for each process for each sublayer of the soil column and for each month of the year. Table 5.1 lists the possible components that would be in the mass

distribution table of the output file and the order in which they would be given. The pollutant mass is printed for each sublayer from the surface to the bottom of the soil column. If a model component in a particular sublayer is 0.0 for each month of the current year, it will not be printed in order to conserve space in the file. For example, washload was not included in the simulation listed in Appendix B, and thus the line that would be labeled "IN WASHLD," that is, the mass of the chemical in µg lost via soil erosion, is not printed.

If there is more than one sublayer in the first layer (upper soil zone), then the output for the second sublayer follows and the order of the parameters and their definitions are the same as given in Table 5.1. However, the first three components listed in Table 5.1 (i.e., "SUR. RUNOFF," "IN WASHLOAD," and "VOLATILIZED") apply only to the uppermost sublayer of the first layer (upper soil zone). The fourth component listed in Table 5.1 (i.e., "DIFFUSED UP") applies to all sublayers except the uppermost sublayer of the first layer (upper soil zone). Likewise, this table continues for each layer (and sublayer) down through the soil column.

If all results for all components of a layer (sublayer) are 0.0 for the year, then the only label printed is the number of the sublayer (e.g., for the year 1 results shown in Appendix B, "SUBLAYER 3" in the "SOIL ZONE 3" had no components listed signifying that the pollutant had not reached this sublayer yet during the first year). When the pollutant reaches the bottom of the soil column (the last sublayer of the "LOWER SOIL ZONE"), the last component printed in the mass distribution table is the mass of pollutant in µg that leaves the unsaturated zone and enters the groundwater (labeled "GWR. RUNOFF").

Table 5.1
Pollutant Mass (µg) Distribution Table in the Output File

Process Label	*Definition*
SUR. RUNOFF	Mass of the pollutant in the surface runoff (first sublayer only).
IN WASHLOAD	Mass of the pollutant lost via soil erosion (first sublayer only).
VOLATILIZED	Mass of pollutant volatilized to air from the first sublayer (first sublayer only).
DIFFUSED UP	Mass of pollutant diffused upward from the layer (sublayer) to the layer (sublayer) above it.
DEGRAD MOIS	Mass of pollutant degraded in the soil moisture phase.
DEGRAD SOIL	Mass of pollutant degraded in the soil adsorbed phase.
HYDROL MOIS	Mass of pollutant degraded due to hydrolysis in the soil moisture phase.
HYDROL SOIL	Mass of pollutant degraded due to hydrolysis in the adsorbed soil phase.
HYDROL CEC	Mass of pollutant degraded due to hydrolysis of the mass of the pollutant immobilized by cation exchange.
OTHER SINKS	This is the value input by the user for SINK1 (or 2, 3, L depending on the layer), in µg/cm^2 , in the application input file multiplied by the surface area and divided by the number of sublayers in the layer.
OTHER TRANS	This is the value input by the user for TRANS1 (or 2,3,L depending on the layer), in µg/cm^2 , in the application input file multiplied by the surface area and divided by the number of sublayers in the layer.
IN SOIL MOIS	Mass of pollutant in the soil moisture phase.
ADS ON SOIL	Mass of pollutant in the soil adsorbed phase.
IN SOIL AIR	Mass of pollutant in the soil air phase.
PURE PHASE	Mass of the pollutant in the pure phase; will be nonzero only if the pollutant concentration in the soil moisture phase exceeds the solubility of the chemical.
COMPLEXED	Mass of the pollutant that is complexed.
IMMOBIL CEC	Mass of pollutant immobilized by cation exchange.
GWR. RUNOFF	Mass of pollutant that leaves the unsaturated zone and enters the groundwater (lowest sublayer only).

Following the pollutant mass distribution table is a table of the monthly pollutant concentrations for each chemical phase for each sublayer of each major soil layer (see Appendix B). The concentrations are printed for each sublayer from the surface to the bottom of the soil column. Table 5.2 lists the possible phases and their labels that would appear in the table in the output file. Again, if all concentrations for a particular phase are 0.0 for each month of the entire year, they are not printed. The pure phase concentration will always be 0.0 unless the simulated pollutant concentration in the soil moisture exceeds the solubility of the

chemical. If this happens, the model sets the soil moisture concentration to the solubility (the %SOLUBILITY defined in Table 5.2 will be 100.0), and the excess chemical is assumed to be in the pure phase. Note that transport of the chemical in the pure phase is not considered; the pure phase is treated as an immobile storage term and the mass of the chemical in this phase is used as input to the same layer in the next time step.

Table 5.2
Pollutant Concentration Table in the Output File

Phase Label	*Definition*
MOISTURE	Pollutant concentration in the soil moisture phase in µg/mL.
%SOLUBILITY	Not a concentration, but is the soil moisture concentration divided by the solubility for the chemical that was input in the chemical input file, multiplied by 100 to give %.
ADSORBED	Pollutant concentration in the soil adsorbed phase in µg/g.
SOIL AIR	Pollutant concentration in the soil air phase in µg/mL.
FREE LIGAND	Free ligand concentration in µg/mL.
PURE PHASE	Pollutant concentration in the pure phase in µg/ml.

At the end of this table the pollutant depth in cm is printed (labeled "POL DEP CM"). This depth is calculated from Eq. (11) from Section 3.5.2 and is simply the depth of the leading edge of the pollutant. When the pollutant reaches the groundwater, this depth will always be equal to the depth from the surface to the groundwater table.

5.1.3 Output Of Annual Summary

After the table of concentrations and the pollutant depth for each month are printed, an annual summary report is given (see Appendix B). Definitions in this report are the same as listed above for monthly results, but either a "TOTAL" or an "AVERAGE" is given for each parameter. "TOTAL" is simply the sum of

values given for the 12 months for the parameter listed and "AVERAGE" is the sum for the year divided by 12. The annual summary is organized in the following order:

- ☐ **Total pollutant mass inputs**
- ☐ **Hydrologic cycle components (average or total)**
- ☐ **Total pollutant mass removed from each layer (sublayer)**
- ☐ **Average pollutant concentration distributions for each layer (sublayer)**
- ☐ **Maximum pollutant depth**

Note that the final end-of-the-year pollutant mass in the soil moisture, adsorbed on soil, in soil air, immobilized by cation exchange, complexed, and in the pure phase would be found under the last month of the year (September) in the monthly mass distribution table described in Section 5.1.2.

At the end of this annual report, the maximum depth that the pollutant reaches in meters is given (labeled "MAX. POLL. DEPTH (M)"). This depth will always be the same as printed for the last month of the year (September) just given (see line labeled "POL DEP CM").

Subsequent results given in the output file are as explained in Sections 5.1.2 and 5.1.3 above, given for each year of the simulation.

5.2 Graphing SESOIL Output Report Files

RISKPRO can create bar-chart graphs of SESOIL model results. The graphs may be created for "Concentration vs. Time" for any depth of the soil profile, or "Pollutant Depth vs. Time" which plots the depth of the pollutant front vs. time.

☑ **Step 1** **Select option 3 labeled SESOIL Graphics (SEGRAPH) from the Seasonal Soil Compartment Model Menu and press the ENTER key (See Figure 61).**

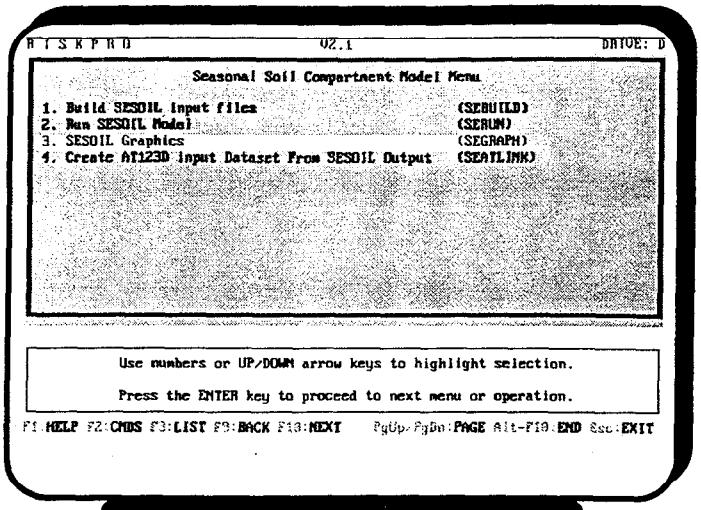
R I S K P R O
V2.1
DRIVE: D
Seasonal Soil Compartment Model Menu
1. Build SESOIL input files (SEBUILD)
2. Run SESOIL Model (SERUN)
3. SESOIL Graphics (SEGRAPH)
4. Create AI123D input Dataset From SESOIL Output (SEAILINK)
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 61
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 62, you are prompted to enter the name of the SESOIL results file (SSOUTxxx.RES) which contains the data needed to create the graphics. It has the same name as the report file for the model run, except with extension ".RES". Press F3 to get a list of files in the catalog. If you don't specify the .RES extension, it will be assumed. The default name shown is the name of the graphics file from the latest SESOIL run.**

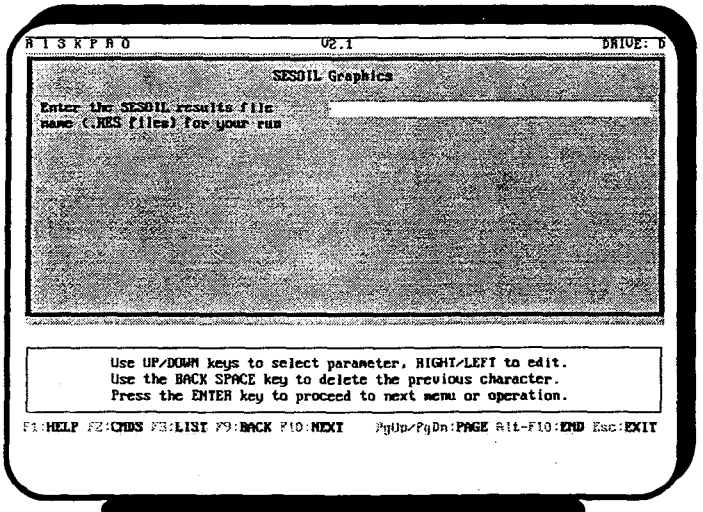
R I S K P R O
V2.1
DRIVE: D
SESOIL Graphics
Enter the SESOIL results file name (.RES files) for your run
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 62
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 3** **As shown in Fig. 63, the <u>SESOIL Output Bar Chart Options</u> menu offers you the following options:**

- ☐ ***OPTION 1*** **allows you to produce a "concentration vs. time" bar chart at any specified soil depth (see Section 5.2.1).**
- ☐ ***OPTION 2*** **allows you to graph a "pollutant depth vs. time" bar chart (see Section 5.2.2).**

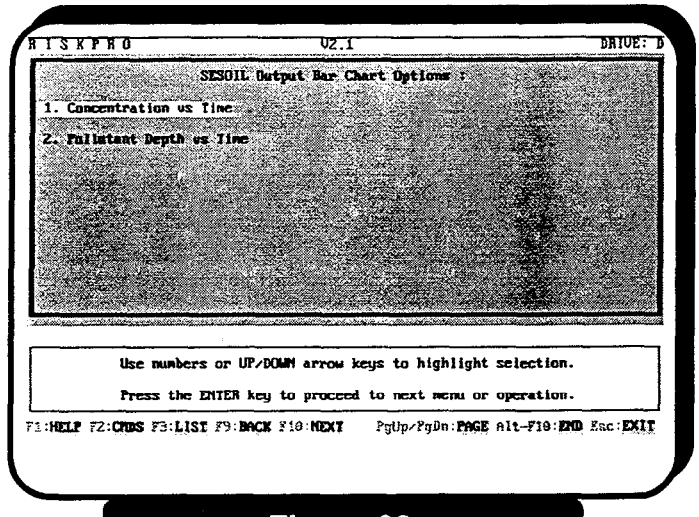
RISKPRO V2.1 DRIVE: D
SESOIL Output Bar Chart Options :
1. Concentration vs Time
2. Pollutant Depth vs Time
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CHBS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 63
Screen courtesy of General Sciences Corporation's RISKPRO+, Version 2.1© copyright 1991.

5.2.1 Graphing "Concentration Vs. Time"

☑ **Step 1** **Choose the first option from Fig. 63 and press the ENTER key. As shown in Fig. 64, you will be offered three menu options where:**

- ☐ ***OPTION 1*** **plots the pollutant concentration dissolved in the soil moisture (dissolved phase).**
- ☐ ***OPTION 2*** **plots the pollutant concentration adsorbed to the soil particles (adsorbed phase).**
- ☐ ***OPTION 3*** **plots the pollutant concentration in the soil air pores (vapor phase).**

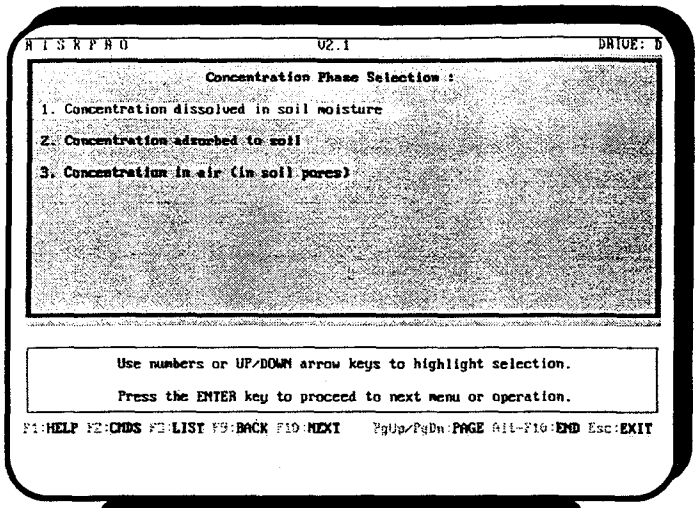
RISKPRO V2.1 DRIVE: D
Concentration Phase Selection :
1. Concentration dissolved in soil moisture
2. Concentration adsorbed to soil
3. Concentration in air (in soil pores)
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 64
Screen courtesy of General Sciences Corporation's RISKPRO©, Version 2.1© copyright 1991.

☑ **Step 2** **Choose any of the three options from Fig. 64 and press the ENTER key.**

☑ **Step 3** **Next, enter the depth from the soil surface in cm (see Fig. 65) and press the ENTER key.**

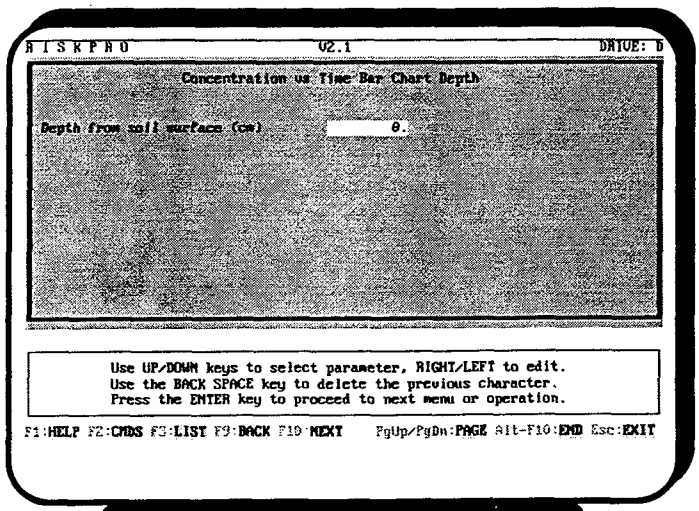
RISKPRO V2.1 DRIVE: D
Concentration vs Time Bar Chart Depth
Depth from soil surface (cm) 0.
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 65
Screen courtesy of General Sciences Corporation's RISKPRO©, Version 2.1© copyright 1991.

❑ ***Technical Note:*** *This depth is the depth from the soil surface for the "concentration vs. time" bar chart in cm. The concentration values in the sublayer at the specified depth will be used for this plot routine. Entering a zero depth here will use the concentration values in the uppermost sublayer of the top soil layer.*

☑ **Step 4** **As shown in Fig. 66, you will be given two options in the time increment menu where:**

☐ *OPTION 1* **uses a time increment of one month for the bar chart.**

☐ *OPTION 2* **uses a time increment of one year for the bar chart.**

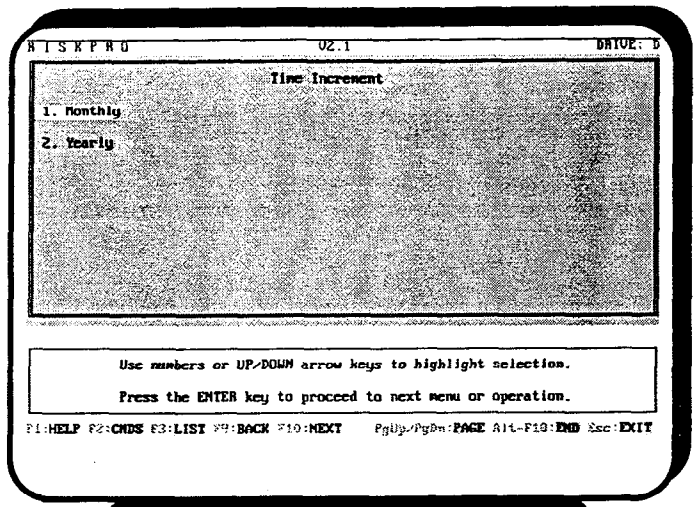
RISKPRO V2.1 DRIVE: D
Time Increment
1. Monthly
2. Yearly
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 66
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☐ *Side Note:* *Pressing the ENTER key at Step 6 uses the defaults listed in the menu, and you will go to Step 12. Otherwise, arrow down to the next step.*

☑ **Step 5** **Select either option and press the ENTER key to proceed to the *Bar Chart Title* menu as shown in Fig. 67. Here you are given several options to enhance your chart .**

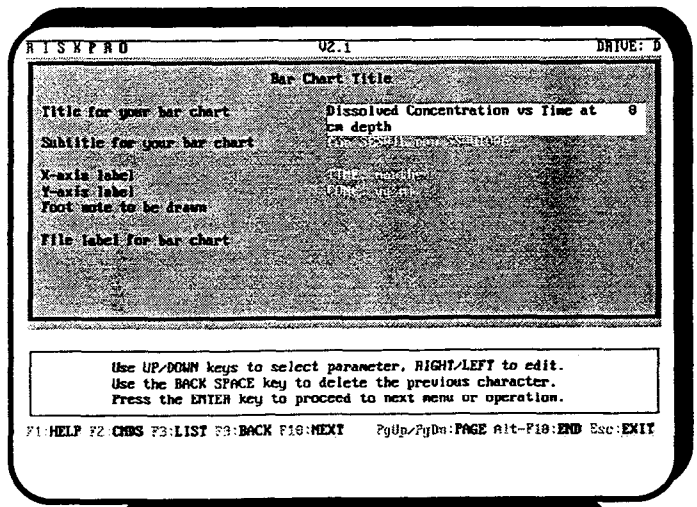
RISKPRO V2.1 DRIVE: D
Bar Chart Title
Title for your bar chart
Dissolved Concentration vs Time at 0 cm depth
Subtitle for your bar chart
X-axis label
Y-axis label
Foot note to be drawn
File label for bar chart
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 67
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 6** **Highlight the option labeled *Title for your bar chart* and enter a title for the bar chart. This title will appear above the bar chart.**

☑ **Step 7** **Highlight the option labeled *Subtitle for your bar chart* and enter a subtitle for the bar chart. This entry will appear under the title, in smaller characters.**

☑ **Step 8** **Highlight the X-axis label option. This label will appear below the X-axis. You should include the units.**

☑ **Step 9** **Highlight and enter the Y-axis label option. This label will appear below the Y-axis. You should include the units.**

☑ **Step 10** **Highlight the option labeled *Foot note to be drawn*. A foot note for the bar chart can be entered. This is optional, and may be left blank.**

☑ **Step 11** **For the final option, enter a descriptive label for the bar chart and press the ENTER key. This entry is required for cataloging the output file and will be displayed by the RISKPRO Catalog Manager for identification purposes.**

☑ **Step 12** **At this point, you should see a graph created by the RISKPRO system. Press the ENTER key to return to the *Seasonal Soil Compartment Model Menu* (shown in Fig. 61).**

☐ ***Technical Note:*** *To view or graph any of the bar chart files, use the Catalog manager in RISKPRO. See Section 4.2 of the RISKPRO documentation (General Science Corporation, 1990).*

5.2.2 Graphing "Pollutant Depth Vs. Time"

☑ **Step 1** **As shown in Fig. 68, choose the *Pollutant Depth vs. Time* option and press the ENTER key. This option produces a bar chart of the depth of the pollutant front vs. time.**

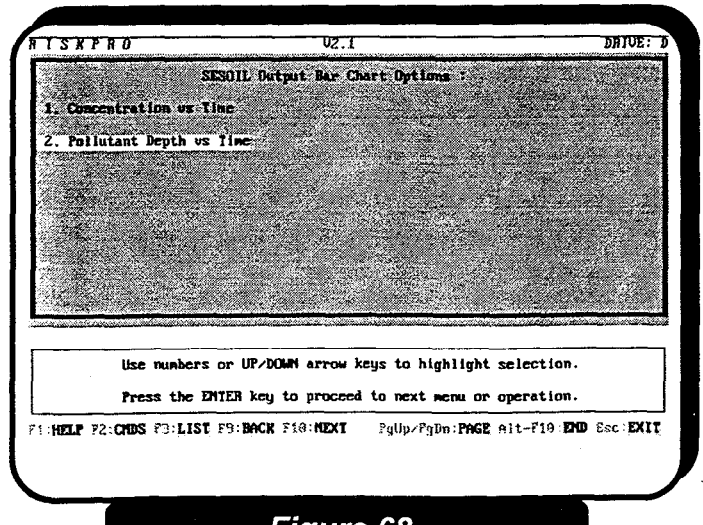
RISKPRO V2.1 DRIVE: D
SESOIL Output Bar Chart Options :
1. Concentration vs Time
2. Pollutant Depth vs Time
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 68
Screen courtesy of General Sciences Corporation's RISKPRO®, Version 2.1© copyright 1991.

☑ **Step 2** **As shown in Fig. 69, you will be given two options in the time increment menu where:**

- ☐ *OPTION 1* **uses a time increment of one month for the bar chart.**
- ☐ *OPTION 2* **uses a time increment of one year for the bar chart.**

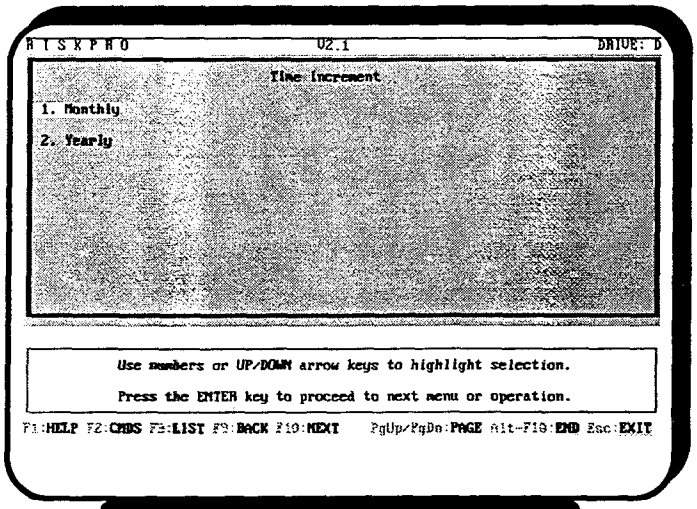
RISKPRO V2.1 DRIVE: D
Time Increment
1. Monthly
2. Yearly
Use numbers or UP/DOWN arrow keys to highlight selection.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 69
Screen courtesy of General Sciences Corporation's RISKPRO©, Version 2.1© copyright 1991.

☑ **Step 3** **Select either option and press the ENTER key to proceed to the *Bar Chart Title* menu as shown in Fig. 70. Here you are given several options to enhance your chart .**

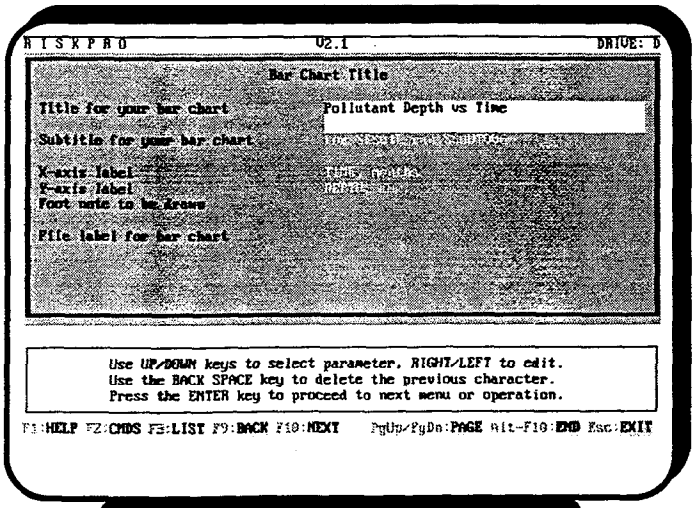
RISKPRO V2.1 DRIVE: D
Bar Chart Title
Title for your bar chart
Pollutant Depth vs Time
Subtitle for your bar chart
X-axis label
Y-axis label
Foot note to be drawn
File label for bar chart
Use UP/DOWN keys to select parameter, RIGHT/LEFT to edit.
Use the BACK SPACE key to delete the previous character.
Press the ENTER key to proceed to next menu or operation.
F1:HELP F2:CMDS F3:LIST F9:BACK F10:NEXT PgUp/PgDn:PAGE Alt-F10:END Esc:EXIT

Figure 70
Screen courtesy of General Sciences Corporation's RISKPRO©, Version 2.1© copyright 1991.

☐ ***Side Note:***
Pressing the ENTER key at Step 4 uses the defaults listed in the menu, and you will go to Step 10. Otherwise, arrow down to the next step.

☑ **Step 4** **Highlight the option labeled *Title for your bar chart* and enter a title for the bar chart. This title will appear above the bar chart.**

☑ **Step 5** **Highlight the option labeled *Subtitle for your bar chart* and enter a subtitle for the bar chart. This entry will appear under the title, in smaller characters.**

☑ **Step 6** **Highlight the X-axis label option. This label will appear below the X-axis. You should include the units.**

☑ **Step 7** **Highlight and enter the Y-axis label option. This label will appear below the Y-axis. You should include the units.**

☑ **Step 8** **Highlight the option labeled *Foot note to be drawn* . A foot note for the bar chart can be entered. This is optional, and may be left blank.**

☑ **Step 9** **For the final option enter a descriptive label for the bar chart and press the ENTER key. This entry is required for cataloging the output file and will be displayed by the RISKPRO Catalog Manager for identification purposes.**

☑ **Step 10** **At this point, you should see a graph created by the RISKPRO system. Press the ENTER key to return to the *Seasonal Soil Compartment Model Menu* (shown in Fig. 61).**

APPENDIX

A

Data Input Examples

An Example Of A Climate Data File

The weather station at Milwaukee, Wisconsin was selected from the climate database file for this example. This selection created the following climate data file.

CLIMATE INPUT DATA FILE

```
 1 MILWAUKEE WSO AP
       ****  YEAR 1  ****
TA      11.27  3.05 -3.94 -6.50 -4.83  0.38  7.94 13.55 19.16 21.88 21.38 16.88
NN       0.50  0.75  0.75  0.70  0.70  0.70  0.65  0.60  0.60  0.50  0.50  0.50
S        0.70  0.75  0.80  0.80  0.80  0.70  0.70  0.70  0.70  0.70  0.70  0.70
A        0.17  0.21  0.30  0.33  0.30  0.29  0.19  0.17  0.17  0.17  0.17  0.17
REP      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
MPM      5.52  5.29  5.39  4.19  3.52  6.55  8.71  6.91  8.96  9.08  7.94  7.07
MTR      0.45  0.51  0.57  0.54  0.53  0.54  0.49  0.39  0.33  0.31  0.27  0.35
MN       4.02  4.50  4.38  3.48  3.00  5.05  6.31  5.88  6.05  5.40  5.62  4.55
MT      30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40
 999 END OF FILE
```

An Example Of A Soil Data File

To create this file the following values were entered:

RS - Bulk Density (g/cm^3)= 1.7
K1 - Intrinsic Permeability (cm^2) = 0.1 x 10-7
C - Soil Disconnectedness Index (-) = 4.0
N - Effective porosity (-) = 0.25
OC - Organic Carbon Content (%) = .50
CEC - Cation Exchange Cap. (meq/100g) = 0.0
FRN - Freundlich Exponent = 1.

SOIL INPUT DATA FILE

```
  1 SAND
      -  RS,K1,C,N,OC              1.70 .10E-07   4.00    0.25    0.50
      -  CEC,FRN                   0.00   1.00
999 END OF FILE
```

An Example Of A Chemical Data File

For the creation of this file the chemical benzene was chosen with the following parameters:

SL - Solubility in water = 1780 (ug/ml)
DA - Air Diffusion Coefficient = .0770 (cm^2/sec)
H - Henrys Law Constant = .00555 (m3-atm/mol)
KOC - OC Adsorption Coefficient = 31 (ug/g-oc)/(ug/ml)
K_d - Soil Partition Coefficient = 0 (ug/g)/(ug/ml)
MWT - Molecular Weight = 78.11 (g/mole)

Note : all other parameters VAL, KNH, KBH, KAH, KDEL, KDES, SK, B, and MWTLIG are set to zero.

CHEMICAL INPUT DATA FILE

```
  1 BENZENE


     - SL,DA,H,KOC,K              1780.00  0.0770.00555  31.00    0.00
     - MWT,VAL,KNH,KBH,KAH          78.11    0.00   0.00   0.00    0.00
     - KDEL,KDES,SK,B,MWTLIG         0.00    0.00   0.00   0.00    0.00
999 END OF FILE
```

An Example Of An Application Data File

For this file the following values were entered:

ILYS - No. of soil layers (2:4) = 4
AR - Application area = 100,000(cm^2)
LAT - Latitude of site (deg) 42.95 degrees
ISPILL - Spill index (0 or 1) = 0

D1 - Upper layer thickness = 200 (cm).
D2 - Second layer thickness = 200 (cm).
D3 - Third layer thickness = 400 (cm).
D4 - Lower layer thickness = 15 (cm).
NSUB1 - # sublayers in upper layer = 1
NSUB2 - # sublayers in 2nd layer = 1
NSUB3 - # sublayers in 3rd layer = 10
NSUB4 - # sublayers in lower layer = 1

PH1 - pH of upper layer (0:14)= 7.
PH2 - pH of second layer (0:14)= 7.
PH3 - pH of third layer (0:14)= 7.
PH4 - pH of lower layer (0:14)= 7.
K11 - Perm. of upper layer = 0(cm^2)
K12 - Perm. of 2nd layer = 0(cm^2)
K13 - Perm. of 3rd layer = 0(cm^2)
K14 - Perm. of lower layer = 0(cm^2)
KDEL2 - Ratio of KDEL layer 2 to 1 = 1.
KDEL3 - Ratio of KDEL layer 3 to 1 = 1.
KDEL4 - Ratio of KDEL layer 4 to 1 = 1.
KDES2 - Ratio of KDES layer 2 to 1 = 1.
KDES3 - Ratio of KDES layer 3 to 1 = 1.
KDES4 - Ratio of KDES layer 4 to 1 = 1.
OC2 - Ratio of OC layer 2 to 1 = 1.
OC3 - Ratio of OC layer 3 to 1 = 1.
OC4 - Ratio of OC layer 4 to 1 = 1.
CEC2 - Ratio of CEC layer 2 to 1 = 1.
CEC3 - Ratio of CEC layer 3 to 1 = 1.
CEC4 - Ratio of CEC layer 4 to 1 = 1.
FRN2 - Ratio of FRN layer 2 to 1 = 1.
FRN3 - Ratio of FRN layer 3 to 1 = 1.
FRN4 - Ratio of FRN layer 4 to 1 = 1.
ADS2 - Ratio of ADS layer 2 to 1 = 1.
ADS3 - Ratio of ADS layer 3 to 1 = 1.
ADS4 - Ratio of ADS layer 4 to 1 = 1.

❑ *Note:* ***A note on the pollutant input parameters:***

Remember that POLIN is a monthly pollutant load (mass per unit area) that enters the top sublayer of the layer you have chosen for loading.

If an initial soil-sorbed concentration of 50 ug/g (ppm) is desired in layer 2 (soil depth of 200-400 cm), the POLIN would be 17000 ug/cm^2/month in the first month (October), and 0.0 thereafter. POLIN was calculated from the following equation:

$$POLIN = CONC * L * RS$$

where:

POLIN is the pollutant load to apply in ug/cm^2/month,

CONC is the concentration sorbed to the soil in ug/g or ppm,

L is the thickness of the sublayer in centimeters which the pollutant is applied (200 cm here), and

RS is the bulk density of the soil in g/cm^3 (1.7 g/cm^3 here).

Note that ISPILL is always 0 for any layer below the first layer so in this case 1.7E9 ug (17000 ug/cm^2 multiplied by the area AR, which is 1.0E5 cm^2) of benzene was loaded into the second layer in the first month. This mass is divided by the number of time steps per month (30) and added to the second layer in equal amounts for each time step throughout the month.

Example Of An Application Data File continued.....

APPLICATION INPUT DATA FILE

```
1 DEFAULT APPLIC DATA
 -ILYS,IYRS,AR,L,ISPILL                    4.00    1.00100000.   42.95  0
 -D1,D2,D3,D4,NSUBL1 to NSUBL4           200.00 200.00 400.00   15.00  1  1 10  1
 -PH1,PH2,PH3,PH4                          7.00   7.00   7.00    7.00
 -K11,K12,K13,K14                          0.00   0.00   0.00    0.00
 -KDEL MULTIPLIERS                         1.00   1.00   1.00
 -KDES MULTIPLIERS                         1.00   1.00   1.00
 -OC MULTIPLIERS                           1.00   1.00   1.00
 -CEC MULTIPLIERS                          1.00   1.00   1.00
 -FRN MULTIPLIERS                          1.00   1.00   1.00
 -ADS MULTIPLIERS                          1.00   1.00   1.00

                **** LAYER 1 **  YEAR 1 ****
POLIN1    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS1    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK1     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG1      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF1     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
ISRM      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ASL       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00

                **** LAYER 2 **  YEAR 1 ****
POLIN2 17000.   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF2     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00

                **** LAYER 3 **  YEAR 1 ****
POLIN3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK3     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG3      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF3     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00

                **** LAYER 4 **  YEAR 1 ****
POLIN4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK4     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG4      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF4     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
```

Input Data File Continued Next Page.....

APPLICATION INPUT DATA FILE
Continued

```
                **** LAYER 1 **  YEAR 2 ****
POLIN1    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS1    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK1     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG1      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF1     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
ISRM      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ASL       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00

                **** LAYER 2 **  YEAR 2 ****
POLIN2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF2     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00

                **** LAYER 3 **  YEAR 2 ****
POLIN3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK3     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG3      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF3     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00

                **** LAYER 4 **  YEAR 2 ****
POLIN4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK4     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG4      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF4     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
                999 END OF FILE
```

An Example Of A Washload Data File (Optional)

This is an example of a washload data file. <u>This input data file was not used for the simulation run listed in Appendix B</u>.

WASHLOAD INPUT DATA FILE

```
1 DEFAULT WASHLOAD DATA - (CLINTON, MA)                    1
ARW,SLT,SND,CLY,SLEN,SLP          10000.0    0.20    0.66    0.146279.00 0.0267

                **MONTHLY DATA**  YR 1
KSOIL     0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23
CFACT     0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26
PFACT     1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
NFACT    0.030 0.030 0.030 0.030 0.030 0.030 0.030 0.030 0.030 0.030 0.030 0.030
999 END OF FILE
```

APPENDIX

B

Output Report Example

To conserve space, only results for the first year of the simulation are printed. In addition, the output report example shown below has been enhanced with bold type and centering formats for certain title headings . An actual SESOIL output file would have a different type set and format type.

An Example of a SESOIL Output Report

```
                    ********************************************************************************************

1

 ***************************************************************************************************************
 *****                                                                                                     *****
 ***** SESOIL-84 :  SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS               *****
 *****                                                                                                     *****
 ***** DEVELOPERS:  M. BONAZOUNTAS,ARTHUR D. LITTLE INC.  ,(617)864-5770,X5871                            *****
 *****             J. WAGNER     ,DIS/ADLPIPE, INC.       ,(617)492-1991,X5820                          *****
 *****                                                                                                     *****
 ***** MODIFIED EXTENSIVELY BY:                                                                           *****
 ***** D.M. HETRICK                                                                                       *****
 ***** OAK RIDGE NATIONAL LABORATORY                                                                      *****
 ***** (615) 576-7556                                                                                     *****
 ***** VERSION    :  SEPTEMBER 1986                                                                       *****
 *****                                                                                                     *****
 ***************************************************************************************************************

                          ********* MONTHLY SESOIL MODEL OPERATION ******
                                  MONTHLY SITE SPECIFIC SIMULATION

                    REGION          :       MILWAUKEE WSO AP
                    SOIL TYPE       :       SAND
                    COMPOUND        :       Benzene
                    WASHLOAD DATA   :
                    APPLICATION AREA:       DEFAULT APPLIC DATA


                                      GENERAL INPUT PARAMETERS
                                    ==============================

                                       -- SOIL INPUT PARAMETERS --

                      SOIL DENSITY (G/CM**3):                                    1.70
                      INTRINSIC PERMEABILITY (CM**2):                            .100E-07
                      DISCONNECTEDNESS INDEX (-):                                4.00
                      POROSITY (-):                                              .250
                      ORGANIC CARBON CONTENT (%):                                .500
                      CATION EXCHANGE CAPACITY (MILLI EQ./100G DRY SOIL):        .000
                      FREUNDLICH EXPONENT (-):                                   1.00
```

1

-- CHEMICAL INPUT PARAMETERS --

SOLUBILITY (UG/ML):	.178E+04
DIFFUSION COEFFICIENT IN AIR (CM**2/SEC):	.770E-01
HENRYS LAW CONSTANT (M**3-ATM/MOLE):	.555E-02
ADSORPTION COEFFICIENT ON ORGANIC CARBON(KOC):	31.0
ADSORPTION COEFFICIENT ON SOIL (K):	.000
MOLECULAR WEIGHT (G/MOL):	78.1
VALENCE (-):	.000
NEUTRAL HYDROLYSIS CONSTANT (/DAY):	.000
BASE HYDROLYSIS CONSTANT (L/MOL-DAY):	.000
ACID HYDROLYSIS CONSTANT (L/MOL-DAY):	.000
DEGRADATION RATE IN MOISTURE (/DAY):	.000
DEGRADATION RATE ON SOIL (/DAY):	.000
LIGAND-POLLUTANT STABILITY CONSTANT (-):	.000
NO. MOLES LIGAND/MOLE POLLUTANT (-):	.000
LIGAND MOLECULAR WEIGHT (G/MOL):	.000

-- APPLICATION INPUT PARAMETERS --

NUMBER OF SOIL LAYERS:			4	
YEARS TO BE SIMULATED:			3	
AREA (CM**2):			0.100E+06	
APPLICATION AREA LATITUDE (DEG.):			43.0	
SPILL (1) OR STEADY APPLICATION (0):			0	
DEPTHS (CM):	0.20E+03	0.20E+03	0.40E+03	15.
NUMBER OF SUBLAYERS/LAYER	1	1	10	1
PH (CM):	7.0	7.0	7.0	7.0
INTRINSIC PERMEABILITIES (CM**2):	0.00	0.00	0.00	0.00
KDEL RATIOS (-):	1.0	1.0	1.0	
KDES RATIOS (-):	1.0	1.0	1.0	
OC RATIOS (-):	1.0	1.0	1.0	
CEC RATIOS (-):	1.0	1.0	1.0	
FRN RATIOS(-):	1.0	1.0	1.0	
ADS RATIOS(-):	1.0	1.0	1.0	

1

YEAR - 1
MONTHLY INPUT PARAMETERS

-- CLIMATIC INPUT PARAMETERS --

	OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP
TEMP. (DEG C)	11.270	3.050	-3.940	-6.500	-4.830	0.380	7.940	13.550	19.160	21.880	21.380	16.880
CLOUD CVR (FRAC.)	0.500	0.750	0.750	0.700	0.700	0.700	0.650	0.600	0.600	0.500	0.500	0.500
REL. HUM. (FRAC.)	0.700	0.750	0.800	0.800	0.800	0.700	0.700	0.700	0.700	0.700	0.700	0.700
ALBEDO (-)	0.170	0.210	0.300	0.330	0.300	0.290	0.190	0.170	0.170	0.170	0.170	0.170
EVAPOT. (CM/DAY)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRECIP. (CM)	5.520	5.290	5.390	4.190	3.520	6.550	8.710	6.910	8.960	9.080	7.940	7.070
M.TIME RAIN(DAYS)	0.450	0.510	0.570	0.540	0.530	0.540	0.490	0.390	0.330	0.310	0.270	0.350
M. STORM NO. (-)	4.020	4.500	4.380	3.480	3.000	5.050	6.310	5.880	6.050	5.400	5.620	4.550
M. SEASON (DAYS)	30.400	30.400	30.400	30.400	30.400	30.400	30.400	30.400	30.400	30.400	30.400	30.400

-- POLLUTANT INPUT PARAMETERS --

POL. INP-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-1	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
SURFACE RUNOFF MULT.	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
POL. IN RAIN (FRAC-SL)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

POL. INP-2 (UG/CM**2)	1.70E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-2	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

POL. INP-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-3	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

POL. INP-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-L	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

1

YEAR - 2
MONTHLY INPUT PARAMETERS
==========

CLIMATIC INPUT PARAMETERS ARE SAME AS LAST YEAR
-- POLLUTANT INPUT PARAMETERS --

POL. INP-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-1 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-1	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
SURFACE RUNOFF MULT.	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
POL. IN RAIN (FRAC-SL)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

POL. INP-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-2 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-2	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

POL. INP-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-3 (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-3	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

POL. INP-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
TRNSFORMD-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SINKS-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
LIG.INPUT-L (UG/CM**2)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
VOLATILIZATION MULT.-L	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

1

YEAR - 3
MONTHLY INPUT PARAMETERS
==========

CLIMATIC INPUT PARAMETERS ARE SAME AS LAST YEAR
POLLUTANT INPUT PARAMETERS ARE SAME AS LAST YEAR

YEAR - 1
MONTHLY RESULTS (OUTPUT)

-- HYDROLOGIC CYCLE COMPONENTS --

	OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP
MOIS. IN L1 (%)	4.901	5.576	6.201	6.101	5.576	5.676	5.551	4.951	5.076	5.076	4.901	4.926
MOIS. BELOW L1 (%)	4.901	5.576	6.201	6.101	5.576	5.676	5.551	4.951	5.076	5.076	4.901	4.926
PRECIPATION (CM)	5.559	5.275	5.424	4.219	3.547	6.572	8.790	6.894	8.886	9.022	7.923	7.035
NET INFILT. (CM)	5.559	5.275	5.424	4.219	3.547	6.572	8.790	6.894	8.886	9.022	7.923	7.035
EVAPOTRANS. (CM)	2.695	0.896	0.304	0.304	0.926	2.644	4.390	3.981	4.563	4.498	4.156	3.472
MOIS. RETEN (CM)	-0.136	0.458	0.424	-0.068	-0.357	0.068	-0.085	-0.407	0.085	0.000	-0.119	0.017
SUR. RUNOFF (CM)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
GRW. RUNOFF (CM)	3.000	3.920	4.695	3.983	2.978	3.860	4.485	3.320	4.238	4.524	3.886	3.547
YIELD (CM)	3.000	3.920	4.695	3.983	2.978	3.860	4.485	3.320	4.238	4.524	3.886	3.547
PAU/MPA (GZU)	1.007	0.997	1.006	1.007	1.008	1.003	1.009	0.998	0.992	0.994	0.998	0.995
PA/MPA (GZ)	1.007	0.997	1.006	1.007	1.008	1.003	1.009	0.998	0.992	0.994	0.998	0.995

-- POLLUTANT MASS INPUT TO COLUMN (UG) --

	OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP
PRECIP.	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
LOAD UPPER	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
LOAD ZONE 2	1.700E+09	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
LOAD ZONE 3	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
LOAD LOWER	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
TOTAL INPUT	1.700E+09	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

0 -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) -- NOTE: IF COMPONENT IS ZERO EACH MONTH, IT IS NOT PRINTED

UPPER SOIL ZONE:
SUBLAYER 1

VOLATILIZED	1.442E+07	5.940E+07	7.712E+07	8.745E+07	9.957E+07	9.386E+07	8.761E+07	8.967E+07	7.826E+07	6.830E+07	6.315E+07	5.749E+07
IN SOIL MOI	2.152E+07	5.141E+07	6.739E+07	7.076E+07	6.593E+07	6.336E+07	5.735E+07	4.848E+07	4.417E+07	3.900E+07	3.413E+07	3.097E+07
ADS ON SOIL	1.157E+08	2.429E+08	2.864E+08	3.056E+08	3.115E+08	2.941E+08	2.722E+08	2.580E+08	2.293E+08	2.024E+08	1.835E+08	1.656E+08
IN SOIL AIR	2.088E+07	4.366E+07	5.113E+07	5.468E+07	5.705E+07	5.292E+07	4.813E+07	4.606E+07	3.986E+07	3.472E+07	3.180E+07	2.904E+07

SOIL ZONE 2:
SUBLAYER 1

DIFFUSED UP	1.877E+08	2.529E+08	1.685E+08	1.363E+08	1.228E+08	1.032E+08	9.638E+07	9.478E+07	7.421E+07	6.326E+07	6.166E+07	5.387E+07
IN SOIL MOI	2.064E+08	1.948E+08	1.896E+08	1.684E+08	1.401E+08	1.318E+08	1.213E+08	9.621E+07	8.484E+07	7.692E+07	6.687E+07	5.944E+07
ADS ON SOIL	1.109E+09	9.206E+08	8.055E+08	7.274E+08	6.619E+08	6.119E+08	5.758E+08	5.120E+08	4.404E+08	3.993E+08	3.595E+08	3.179E+08
IN SOIL AIR	2.003E+08	1.655E+08	1.438E+08	1.302E+08	1.212E+08	1.101E+08	1.018E+08	9.140E+07	7.656E+07	6.849E+07	6.230E+07	5.575E+07

SOIL ZONE 3:
SUBLAYER 1

DIFFUSED UP	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.930E+07	2.185E+07	1.186E+07
IN SOIL MOI	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.808E+06	1.330E+07	1.675E+07	1.367E+07	1.214E+07
ADS ON SOIL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.559E+07	6.904E+07	8.695E+07	7.350E+07	6.491E+07
IN SOIL AIR	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.567E+06	1.200E+07	1.492E+07	1.274E+07	1.138E+07

SUBLAYER 2

IN SOIL MOI	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	5.453E+06	1.009E+07
ADS ON SOIL	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.932E+07	5.396E+07
IN SOIL AIR	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	5.080E+06	9.462E+06

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            SUBLAYER  3
            SUBLAYER  4
            SUBLAYER  5
            SUBLAYER  6
            SUBLAYER  7
            SUBLAYER  8
            SUBLAYER  9
            SUBLAYER 10

      LOWER SOIL ZONE:
            SUBLAYER  1

      -- POLLUTANT CONCENTRATIONS (UG/ML) OR (UG/G) -- NOTE: IF CONCENTRATIONS ARE ZERO FOR EACH MONTH, THEY ARE NOT PRINTED --

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      UPPER SOIL ZONE:
            SUBLAYER  1
MOISTURE     2.195E+01 4.610E+01 5.434E+01 5.799E+01 5.911E+01 5.581E+01 5.166E+01 4.896E+01 4.351E+01 3.841E+01 3.482E+01 3.143E+01
%SOLUBILITY 1.233E+00 2.590E+00 3.053E+00 3.258E+00 3.321E+00 3.135E+00 2.902E+00 2.751E+00 2.444E+00 2.158E+00 1.956E+00 1.766E+00
ADSORBED     3.402E+00 7.145E+00 8.422E+00 8.988E+00 9.162E+00 8.650E+00 8.007E+00 7.589E+00 6.744E+00 5.953E+00 5.397E+00 4.871E+00
SOIL AIR     5.194E+00 1.124E+01 1.360E+01 1.447E+01 1.469E+01 1.369E+01 1.237E+01 1.149E+01 1.000E+01 8.714E+00 7.911E+00 7.234E+00


      SOIL ZONE 2:
            SUBLAYER  1
MOISTURE     2.105E+02 1.747E+02 1.528E+02 1.380E+02 1.256E+02 1.161E+02 1.093E+02 9.716E+01 8.356E+01 7.576E+01 6.822E+01 6.032E+01
%SOLUBILITY 1.183E+01 9.814E+00 8.587E+00 7.755E+00 7.056E+00 6.523E+00 6.138E+00 5.458E+00 4.695E+00 4.256E+00 3.832E+00 3.389E+00
ADSORBED     3.263E+01 2.708E+01 2.369E+01 2.140E+01 1.947E+01 1.800E+01 1.694E+01 1.506E+01 1.295E+01 1.174E+01 1.057E+01 9.350E+00
SOIL AIR     4.982E+01 4.259E+01 3.825E+01 3.443E+01 3.121E+01 2.849E+01 2.617E+01 2.280E+01 1.921E+01 1.719E+01 1.550E+01 1.389E+01


      SOIL ZONE 3:
            SUBLAYER  1
MOISTURE     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 2.428E+01 6.550E+01 8.250E+01 6.973E+01 6.159E+01
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.364E+00 3.680E+00 4.635E+00 3.917E+00 3.460E+00
ADSORBED     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 3.763E+00 1.015E+01 1.279E+01 1.081E+01 9.546E+00
SOIL AIR     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 5.696E+00 1.506E+01 1.872E+01 1.584E+01 1.418E+01
            SUBLAYER  2
MOISTURE     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 2.781E+01 5.119E+01
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.563E+00 2.876E+00
ADSORBED     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 4.311E+00 7.935E+00
SOIL AIR     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 6.319E+00 1.178E+01


      LOWER SOIL ZONE:

POL DEP CM   3.128E+02 3.258E+02 3.397E+02 3.508E+02 3.599E+02 3.750E+02 3.948E+02 4.079E+02 4.231E+02 4.390E+02 4.528E+02 4.653E+02
                                                    1
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YEAR - 1
ANNUAL SUMMARY REPORT
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-- TOTAL INPUTS (UG) --

UPPER SOIL ZONE	0.000E+00
SOIL ZONE 2	1.700E+09
SOIL ZONE 3	0.000E+00
LOWER SOIL ZONE	0.000E+00

-- HYDROLOGIC CYCLE COMPONENTS --

AVERAGE SOIL MOISTURE ZONE 1 (%)	5.376
AVERAGE SOIL MOISTURE BELOW ZONE 1 (%)	5.376
TOTAL PRECIPITATION (CM)	79.145

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                        TOTAL INFILTRATION (CM)                    79.145
                        TOTAL EVAPOTRANSPIRATION (CM)              32.828
                        TOTAL SURFACE RUNOFF (CM)                   0.000
                        TOTAL GRW RUNOFF (CM)                      46.435
                        TOTAL MOISTURE RETENTION (CM)              -0.118
                        TOTAL YIELD (CM)                           46.435
 0          -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) -- NOTE: IF COMPONENT IS ZERO EACH MONTH, IT IS NOT PRINTED
                              FOR FINAL MASS IN SOIL MOI., ADS. ON SOIL, SOIL AIR, IMMOBIL
                          CEC, COMPLEXED, AND PURE PHASE FOR EACH SUBLAYER, SEE ABOVE (MONTH SEP)
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      UPPER SOIL ZONE:
            SUBLAYER  1
              TOTAL VOLATILIZED                 8.763E+08


      SOIL ZONE 2:
            SUBLAYER  1
              TOTAL DIFFUSED (UP)               1.416E+09


      SOIL ZONE 3:
            SUBLAYER  1
              TOTAL DIFFUSED (UP)               6.301E+07

            SUBLAYER  2
            SUBLAYER  3
            SUBLAYER  4
            SUBLAYER  5
            SUBLAYER  6
            SUBLAYER  7
            SUBLAYER  8
            SUBLAYER  9
            SUBLAYER 10

      LOWER SOIL ZONE:
            SUBLAYER  1

 1          -- AVERAGE POLLUTANT CONCENTRATIONS --  NOTE: ONLY NON-ZERO VALUES ARE PRINTED --


      UPPER SOIL ZONE:
            SUBLAYER  1
                                    SOIL MOISTURE (UG/ML)  4.534E+01
                                    ADSORBED SOIL (UG/G)   7.028E+00
                                    SOIL AIR (UG/ML)       1.088E+01

      SOIL ZONE 2:
            SUBLAYER  1
                                    SOIL MOISTURE (UG/ML)  1.177E+02
                                    ADSORBED SOIL (UG/G)   1.824E+01
                                    SOIL AIR (UG/ML)       2.830E+01
      SOIL ZONE 3:
            SUBLAYER  1
                                    SOIL MOISTURE (UG/ML)  2.530E+01
                                    ADSORBED SOIL (UG/G)   3.921E+00
                                    SOIL AIR (UG/ML)       5.791E+00
            SUBLAYER  2
                                    SOIL MOISTURE (UG/ML)  6.584E+00
                                    ADSORBED SOIL (UG/G)   1.021E+00
                                    SOIL AIR (UG/ML)       1.509E+00
      LOWER SOIL ZONE:

                                    MAX. POLL. DEPTH (M)   4.653E+00
 1
 RESULTS FOR SUBSEQUENT YEARS WOULD FOLLOW HERE.............................
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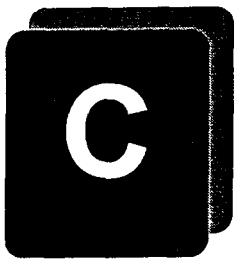
APPENDIX



Error Or Warning Messages

The following lists error or warning messages that are detected by the SESOIL code during operation. Key words are given for the messages in alphabetical order, followed by the error or warning that is printed by the code (the ????? represent a number that is printed by the code). An explanation is given for each.

KEY WORDS	*ERROR OR WARNING*	*EXPLANATION*
Clay Content	FATAL ERROR - CLAY CONTENT (CLY) MUST BE BETWEEN 0 AND 1. IS: ?????	Input for CLY in washload input file is in error.
Cloud Cover (annual)	FATAL ERROR - CLOUD COVER (NN) MUST BE BETWEEN 0. AND 1. IS: ?????	Cloud cover should be a fraction in the ANNUAL input file.
Cloud Cover (monthly)	FATAL ERROR - CLOUD COVER (NN) MUST BE BETWEEN 0. AND 1.	Cloud cover should be a fraction in the CLIMATE input file.
Humidity (Annual)	FATAL ERROR - HUMIDITY (S) MUST BE BETWEEN 0. AND 1. IS: ?????	Humidity should be a fraction in the ANNUAL input file.
Humidity (monthly)	FATAL ERROR - HUMIDITY (S) MUST BE BETWEEN 0. AND 1. IS: ?????	Humidity should be a fraction in the CLIMATE input file.
Hydrology cycle	**** WARNING - PROBLEM IN HYDRO CYCLE: BETA/DELTA GREATER THAN 1., RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION (SEE WRR, P. 716, EQ. (47))	Check hydrology cycle results for reasonableness. See Eagleson (1978), p. 716, for details.
Hydrology cycle	**** WARNING - PROBLEM IN HYDRO CYCLE: BETA GREATER THAN 0.5, RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION	Check input data carefully for errors, especially parameters MTR, MN, and MT.
Hydrology cycle	**** WARNING - PROBLEM IN HYDRO CYCLE MN LESS THAN 1., RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION (SEE WRR, P. 757,EQ. (27)	MN,the mean # of storm events for the month, is less 1; check input (see Eagleson (1978), p. 757 for details).
Hydrology cycle	**** WARNING - PROBLEM IN HYDRO CYCLE: TIME BETWEEN STORMS LESS THAN 2 HRS. RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION (SEE WRR, P. 715, EQ. (39))	Check input data carefully (see Eagleson (1978), p. 715, for details)

KEY WORDS	*ERROR OR WARNING*	*EXPLANATION*
Hydrology cycle	**** WARNING - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP, W SET TO EP	W, the velocity of capillary rise, exceeds the potential evapotranspiration EP in the calculation, which is not allowed. W is set to .99*EP - check the hydrology results for reasonableness.
ILYS (# of layers)	ERROR, ILYS = ????? WHICH IS INCORRECT	The # of layers given in the application data file must be either 2, 3, or 4.
Latitude	FATAL ERROR - LATITUDE (L) MUST BE LESS THAN 90 IS: ?????	Input for latitude is incorrect.
Length of Season (annual)	FATAL ERROR - LENGTH OF SEASON (MT) MUST BE LESS THAN 365 IS: ?????	In ANNUAL data file, length of season must be 365 days or less.
Length of Season (monthly)	FATAL ERROR - LENGTH OF SEASON (MT) MUST BE LESS THAN 31	For monthly simulation, length of season must be less than 31 (see CLIMATE file).
NSUBL1 (# of sublayers in layer 1)	ERROR, NSUBL1 = ????? WHICH IS INCORRECT	The # of sublayers in layer 1 in the APPLICATION file must be at least 0 and less than or equal to 10.
NSUBL2 (# of sublayers in layer 2)	ERROR, NSUBL2 = ????? WHICH IS INCORRECT	The # of sublayers in layer 2 in the APPLICATION file must be at least 0 and less than or equal to 10.
NSUBL3 (# of sublayers in layer 3)	ERROR, NSUBL3 = ????? WHICH IS INCORRECT	The # of sublayers in layer 3 in the APPLICATION file must be at least 0 and less than or equal to 10.

KEY WORDS	*ERROR OR WARNING*	*EXPLANATION*
NSUBLL (# of sublayers in lowest layer)	ERROR, NSUBLL = ????? WHICH IS INCORRECT	The # of sublayers in lowest layer in the APPLICATION file must be at least 0 and less than or equal to 10.
Organic Carbon	FATAL ERROR - SOIL ORGANIC CARBON CONTENT (OC) MUST BE LESS THAN 100. IS: ?????	Input for organic carbon content is in error in the SOIL input file.
Permeability	WARNING - SOIL PERMEABILITY VARYS CONSIDERABLY AMONG LAYERS, SESOIL MAY NOT BE ACCURATE FOR SUCH AN INHOMOGENEOUS COLUMN	Hydrology cycle in SESOIL assumes an homogeneous soil column (it will calculate an average of the permeabilities given in the APPLICATION file).
Permeability	WARNING - SOIL PERMEABILITY (K1) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check permeability in the SOIL input data file.
Permeability (layer 1)	WARNING - SOIL PERMEABILITY (K11) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check permeability for layer 1 in the APPLICATION data file.
Permeability (layer 2)	WARNING - SOIL PERMEABILITY (K12) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check permeability for layer 2 in the APPLICATION data file.
Permeability (layer 3)	WARNING - SOIL PERMEABILITY (K13) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check permeability for layer 3 in APPLICATION data file.
Permeability (last layer)	WARNING - SOIL PERMEABILITY (K1L) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check permeability for the lowest layer in the APPLICATION data file.
Porosity	FATAL ERROR - SOIL POROSITY (N) MUST BE LESS THAN 1. IS: ????	Input for soil porosity is in error in the SOIL input data file.

KEY WORDS	ERROR OR WARNING	EXPLANATION
Rainfall (annual)	WARNING - RAINFALL INPUT FLAG (ASL) IS USUALLY LESS THAN 1. IS: ?????	In ANNUAL data file, check parameter ASL.
Rainfall (monthly)	WARNING - RAINFALL INPUT FLAG (ASL) IS USUALLY LESS THAN 1.	In monthly APPLICATION file, check parameter ASL.
Sand content	FATAL ERROR - SAND CONTENT (SND) MUST BE BETWEEN 0. AND 1. IS: ?????	Input for SND in WASHLOAD data file is in error.
Silt content	FATAL ERROR - SILT CONTENT (SLT) MUST BE BETWEEN 0. AND 1. IS: ?????	Input for SLT in WASHLOAD data file is in error.
SO (Soil moisture)	***** SO OUT OF BOUNDS ***** CANNOT CONTINUE WITH THIS RUN	Can not converge on soil moisture in Subroutine HYDROA - check input data carefully.
Soil Moisture	**** FATAL ERROR - SOIL MOISTURE CALCULATED AS .LE. 0, CHECK FOR EVAPOTRANSPIRATION CLOSE TO OR EXCEEDING ANNUAL PRECIPITATION	Check input data carefully.
Soil Moisture	FATAL ERROR - SOIL MOISTURE (SO) MUST BE BETWEEN 0. AND 100. IS: ?????	Input for soil moisture in ANNUAL input data file is incorrect.
Solubility	WARNING - SOLUBILITY ENTERED AS ZERO, SATURATION CHECKS MAY NOT WORK CORRECTLY	Check solubility in the CHEMICAL input file.
Surface Runoff Flag (Annual)	WARNING - RUNOFF FLAG (ISRA) IS USUALLY LESS THAN 1. IS: ?????	Input for surface runoff flag in the ANNUAL data file should be checked.
Surface Runoff Flag (Monthly)	WARNING - RUNOFF FLAG (ISRM) IS USUALLY LESS THAN 1.	Input for surface runoff flag in the monthly APPLICATION file should be checked.
Volatili-zation (Annual)	WARNING - VOLATILIZATION FLAG (VOLU) IS USUALLY LESS THAN 1. IS: ?????	Input for VOLU in the ANNUAL data file should be checked.

KEY WORDS	*ERROR OR WARNING*	*EXPLANATION*
Volatili-zation (Monthly)	WARNING - VOLATILIZATION FLAGS (VOL1, VOL2, VOL3, VOL4) ARE USUALLY LESS THAN OR EQUAL TO 1.	Input for VOL1, VOL2 VOL3, and VOL4 in the monthly APPLICATION file should be checked.
Washload area	FATAL ERROR - AREA FOR WASHLOAD (ARW) MUST BE ON THE ORDER OF 10**4 OR MORE IS: ?????	Input for ARW in the WASHLOAD data file is in error.

REFERENCES

Bonazountas, M., J. Wagner, and B. Goodwin, Evaluation of Seasonal Soil/Groundwater Pollutant Pathways. EPA Contract No. 68-01-5949 (9), Arthur D. Little, Inc., Cambridge, Massachusetts, 1982.

Bonazountas, M., and J. Wagner (Draft), SESOIL: A Seasonal Soil Compartment Model. Arthur D. Little, Inc., Cambridge, Massachusetts, prepared for the U.S. Environmental Protection Agency, Office of Toxic Substances, 1981, 1984. (Available through National Technical Information Service, publication PB86-112406).

Brinkman, F. E. and J. M. Bellama (editors), Organometals and Organometalloids, Occurrence and Fate in the Environment, ACS Symposium Series 82, American Chemical Society, Washington, D.C., 1978.

Brooks, R. H. and A. T. Corey, Properties of Porous Media Affecting Fluid Flow. Proc. ASCE Journal of the Irrigation and Drainage Division., No. IR 2, Paper 4855, 1966.

Cowan, J. R., Transport of Water in the Soil-Plant-Atmosphere System. J. App. Ecology, Vol. 2, 1965.

Donnigan and Dean, Environmental Exposures from Chemicals, Vol. 1. Edited by W. B. Neely and G. E. Blau, CRC Press, Boca Raton, Fla., p. 100, 1985.

Eagleson, P. S., Climate, Soil, and Vegetation. Water Resources Research 14(5): 705-776, 1978.

Eagleson, P. S. and T. E. Tellers, Ecological Optimality in Water-Limited Natural Soil-Vegetation Systems. 2. Tests and Applications. Water Resources Research 18 (2): 341-354, 1982.

Fairbridge, R. W. and C. W. Finke, Jr. (editors), The Encyclopedia of Soil Science, Part 1. Stroudsburg, PA, Dowden, Hutchinson & Ross, Inc., 646 pp., 1979.

Farmer, W. J., M. S. Yang, J. Letey, and W. F. Spencer, Hexachlorobenzene: Its Vapor Pressure and Vapor Phase Diffusion in Soil. Soil Sci. Soc. Am. J. 44, 676-680, 1980.

Foster, G. R., L. J. Lane, J. D. Nowlin, J. M. Laflen, and R. A. Young, A Model to Estimate Sediment Yield from Field-Sized Areas: Development of Model. Purdue Journal No. 7781, 1980.

Gardner, R. H., A Unified Approach to Sensitivity and Uncertainty Analysis. Proceedings of the Tenth IASTED International Symposium: Applied Simulation and Modelling, San Francisco, California, 1984.

General Sciences Corporation, User's Guide to SESOIL Execution in GEMS. Prepared for USEPA, OTS, Contract No. 68-02-4281, Laurel, MD, 1987.

General Sciences Corporation, Graphical Exposure Modeling System (GEMS) User's Guide. Prepared for USEPA, OTS, Contract No. 68-02-3770, Laurel, MD, 1989.

General Sciences Corporation, RISKPRO User's Guide. General Sciences Corporation, Laurel, Maryland, 1990.

Giesy, J. P., Jr. and J. J. Alberts, Trace Metal Speciation: The Interaction of Metals with Organic Constituents of Surface Waters. In: Proc.of Workshop on The Effects of Trace Elements on Aquatic

Ecosystems, Raleigh, North Carolina, March 23-24, B. J. Ward (editor) 1982. (published as Rept. EPRI EA3329, Feb. 1984)

Grayman, W. M. and P. S. Eagleson, Streamflow Record Length for Modeling Catchment Dynamics. MIT Report No. 114, MIT Department of Civil Engineers, Cambridge, Massachusetts, 1969.

Hamaker, J. W., Decomposition: Quantitative Aspects. In: Organic Chemicals in the Soil Environment, Vol. 1, C. A. I. Goring and J. W. Hamaker (editors), Marcel Dekker, New York, New York, 1972.

Hetrick, D. M., J. T. Holdeman, and R. J. Luxmoore, AGTEHM: Documentation of Modifications to the Terrestrial Ecosystem Hydrology Model (TEHM) for Agricultural Applications. ORNL/TM-7856, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 119 pp., 1982.

Hetrick, D. M., Simulation of the Hydrologic Cycle for Watersheds. Paper presented at Ninth IASTED International Conference, Energy, Power, and Environmental Systems, San Francisco, California, 1984.

Hetrick, D. M., C. C. Travis, P. S. Shirley, and E. L. Etnier, Model Predictions of Watershed Hydrologic Components: Comparison and Verification. Water Resources Bulletin, 22 (5), 803-810, 1986.

Hetrick, D. M. and C. C. Travis, Model Predictions of Watershed Erosion Components. Water Resources Bulletin, 24 (2), 413-419, 1988.

Hetrick, D. M., C. C. Travis, S. K. Leonard, and R. S. Kinerson, Qualitative Validation of Pollutant Transport Components of an Unsaturated Soil Zone Model (SESOIL). ORNL/TM-10672, Oak Ridge National Laboratory, Oak Ridge, TN, 42 pp., 1989.

Hetrick, D. M., A. M. Jarabek, and C. C. Travis, Sensitivity Analysis for Physiologically Based Pharmacokinetic Models. J. of Pharmacokinetics and Biopharmaceutics, 19 (1) 1-20, 1991.

Holton, G. A., C. C. Travis, E. L. Etnier, F. R. O'Connell, D. M. Hetrick, and E. Dixon, Multi-Pathways Screening-Level Assessment of a Hazardous Waste Incineration Facility. ORNL/TM-8652, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 55 pp., 1984.

Holton, G. A., C. C. Travis, and E. L. Etnier, A Comparison of Human Exposure to PCB Emissions from Oceanic and Terrestrial Incineration. Hazardous Waste and Hazardous Materials, 2 (4), 453-471, 1985.

Hornsby, A. G., P. S. C. Rao, W. B. Wheeler, P. Nkedi-Kizza, and R. L. Jones, Fate of Aldicarb in Florida Citrus Soils: Field and Laboratory Studies. In: Proc. of the NWAA/U.S. EPA Conference on Characterization and Monitoring of the Vadose (Unsaturated) Zone, Las Vegas, NV, December 8-10, D. M. Nielsen and M. Curl (editors), 936-958, 1983.

Jones, R. L., P. S. C. Rao, and A. G. Hornsby, Fate of Aldicarb in Florida Citrus Soil: 2. Model Evaluation. In: Proc. of the NWWA/U.S. EPA Conference on Characterization and Modeling of the Vadose (Unsaturated) Zone, Las Vegas, NV, December 8-10, D. M. Nielson and M. Curl (editors), 959-978, 1983.

Jones, R. L., Field, Laboratory, and Modeling Studies on the Degradation and Transport of Aldicarb Residues in Soil and Groundwater. Presented at ACS Symposium on Evaluation of Pesticides in Groundwater, Miami Beach, April 28 - May 1, 1985.

Jones, R. L., Central California Studies on the Degradation and Movement of Aldicarb Residues, (Draft), 28 pp., 1986.

Jury, W. A., W. J. Farmer, and W. F. Spencer, Behavior Assessment Model for Trace Organics in Soil: II. Chemical Classification and Parameter Sensitivity. J. Environ. Qual. 13 (4), 567-572, 1984.

Kincaid, C. T., J. R. Morery, S. B. Yabusaki, A. R. Felmy, and J. E. Rogers, Geohydrochemical Models for Solute Migration. Vol. 2: Preliminary Evaluation of Selected Computer Codes for Modeling Aqueous Solution and Solute Migration in Soils and Geologic Media. EA-3477, Electric Power Research Institute, Palo Alto, California, 1984.

Knisel, W. G. (Editor), CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. Conservation Research Report No. 26, U.S. Department of Agriculture, 1980.

Knisel, W. G., G. R. Foster, and P. A. Leonard, CREAMS: A System for Evaluating Management Practices. Agricultural Management and Water Quality, by Schaller and Bailey, 1983.

Ladwig, K. J. Groundwater Contamination Susceptibility Evaluation, SESOIL Modeling Results, Prepared for Wisconsin Department of Natural Resources, Madison, WI, 1993.

Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt, Handbook of Chemical Property Estimation Methods, Environmental Behavior of Organic Compounds, McGraw-Hill Book Company, New York, New York, 1982.

Melancon, S. M., J. E. Pollard, and S. C. Hern, Evaluation of SESOIL, PRZM, and PESTAN in a Laboratory Column Leaching Experiment. Environ. Toxicol. Chem. 5 (10), 865-878, 1986.

Metzger, B. H. and P. S. Eagleson, The Effects of Annual Storage and Random Potential Evapotranspiration on the One-Dimensional Annual Water Balance. MIT Report No. 251. Massachusetts Institute of Technology, Department of Civil Engineering, Cambridge, Massachusetts 02139, 1980.

Millington, R. J. and J. M. Quirk, Permeability of Porous Solids. Trans. Faraday Soc. 57, 1200-1207, 1961.

Odencrantz, J. E., J. M. Farr, and C. E. Robinson, Levine/Fricke, Inc., A Better Approach to Soil Cleanup Levels Determination. In: Transport Model Parameter Sensitivity for Soil Cleanup Level Determinations Using SESOIL and AT123D in the Context of the California Leaking Underground Fuel Tank Field Manual, Sixth Annual Conference on Hydrocarbon Contaminated Soils: Analysis, Fate, Environmental and Public Health, in Regulations, University of Massachusetts at Amherst, September, 1991.

Odencrantz, J. E., J. M. Farr, and C. E. Robinson, Transport Model Parameter Sensitivity for Soil Cleanup Level Determinations Using SESOIL and AT123D in the Context of the California Leaking Underground Fuel Tank Field Manual. Journal of Soil Contamination , 1 (2), 159-182, 1992.

O'Neill, R. V., R. H. Gardner, and J. H. Carney, Parameter Constraints in a Stream Ecosystem Model: Incorporation of A Priori Information in Monte Carlo Error Analysis. Ecol. Model. 16, 51-65, 1982.

Patterson, M. R., T. J. Sworski, A. L. Sjoreen, M. G. Browman, C. C. Coutant, D. M. Hetrick, B. D. Murphy, and R. J. Raridon, A User's Manual for UTM-TOX, the Unified Transport Model. ORNL-6064, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 434 pp., 1984.

Penman, H. L., Natural Evaporation from Open Water, Bare Soil, and Grass. Proc. Roy. Soc. (London), Series A, 193, 120-145, 1963.

Philip, J. R., Theory of Infiltration. In Advances in Hydroscience, Vol. 5, edited by V. T. Chow, Academic Press, New York, New York, 1969.

Smith, C. N., G. W. Bailey, R. A. Leonard, and G. W. Langdale, Transport of Agricultural Chemicals from Small Upland Piedmont Watersheds. EPA-600/3-78-056, IAG No. IAG-D6-0381, (Athens, GA: U.S. EPA and Watkinsville, GA: USDA), 364 pp., 1978.

Sposito, G., Trace Metals in Contaminated Waters. Environ. Sci. Technol., Vol. 15, 396-403, 1981.

Toy, T. J., A. J. Kuhaida, Jr., and B. E. Munson, The Prediction of Mean Monthly Soil Temperatures from Mean Monthly Air Temperature. Soil Sci., 126, 181-189, 1978.

Travis, C. C., G. A. Holton, E. L. Etnier, C. Cook, F. R. O'Donnell, D. M. Hetrick, and E. Dixon, Assessment of Inhalation and Ingested Population Exposures from Incinerated Hazardous Wastes. Environment International, 12, 533-540, 1986.

Tucker, W. A., C. Huang, and R. E. Dickinson, Environmental Fate and Transport. In: Benzene in Florida Groundwater, An Assessment of the Significance to Human Health. American Petroleum Institute, Washington, D. C., 79-122, 1986.

Van den Honert, T. H., Water Transport in Plants as a Catenary Process. Discuss. Faraday Soc. 3, 1948.

Wagner, J., M. Bonazountas, and M. Alsterberg, Potential Fate of Buried Halogenated Solvents via SESOIL. Arthur D. Little, Inc., Cambridge, Massachusetts, 52 pp., 1983.

Walsh, P. J., L. W. Barnthouse, E. E. Calle, A. C. Cooper, E. D. Copenhaver, E. D. Dixon, C. S. Dudney, G. D. Griffin, D. M. Hetrick, G. A. Holton, T. D. Jones, B. D. Murphy, G. W. Suter, C. C. Travis, and M. Uziel, Health and Environmental Effects Document on Direct Coal Liquefaction - 1983. Prepared for Office of Health and Environmental Research and Office of Energy Research, Department of Energy, ORNL/TM-9287, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 130 pp., 1984.

Watson, D. B. and S. M. Brown, Testing and Evaluation of the SESOIL Model. Anderson-Nichols and Co., Inc., Palo Alto, CA, 155 pp., 1985.

Wischmeier, W. H. and D. D. Smith, Predicting Rainfall Erosion Losses from Cropland - A guide to Conservation Planning. Agricultural Handbook 537, U.S. Department of Agriculture, 58 pp., 1978.

Yalin, Y. S., An Expression for Bedload Transportation. Journal of the Hydraulics Division. Proc. of the American Society of Civil Engineers, 89 (HY3), 221-250, 1963.

Yeh, G. T., AT123D: Analytical Transient One-, Two-, and Three-Dimensional Simulation of Waste Transport in the Aquifer System. ORNL-5602, Oak Ridge National Laboratory, Oak Ridge, TN 37831, 1981 (Available through National Technical Information Service, Publication ORNL-5602/LT).

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